1974

Comparative study: municipal solid waste recovery and incineration using air feed and oxygen feed as combustion mediums

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COMPARATIVE STUDY: MUNICIPAL SOLID WASTE RECOVERY AND INCINERATION USING AIR FEED AND OXYGEN FEED AS COMBUSTION MEDIUMS

by

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A Research Report
Presented to the Graduate Faculty
of Lehigh University
in Candidacy for the Degree of
Master of Science
in
Chemical Engineering
Lehigh University
1974

ACKNOWLEDGEMENTS

For their assistance, I wish to thank students Gregory Gianforcaro, John O'Hara, and David Scholten. For extending financial support to this study, I gratefully acknowledge the Alfred P. Sloane Foundation. Also, for his advice and continued encouragement throughout the course of this project, I sincerely thank Dr. L. A. Wenzel.

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ABSTRACT

A process and economic evaluation has been made of comparable municipal solid waste recovery and incineration systems. The traditional incineration process is supplied with air and a small amount of recycled product gas as the combustion medium, while the other incineration process is supplied with essentially pure oxygen and a large amount of recycled product gas.

From the solid waste recovery process, ferrous metal, paper fiber, glass, and aluminum are extracted for sale. The remaining solid waste is passed into the incinerator with the combustion medium being considered. Thermal and chemical equilibriums obtained within the incinerator have been established through the development and use of digital computer program GARBAGE. Heat from the incinerator is used to generate steam for use in electric power generation. Stack gas is cleaned using electrostatic precipitators before being released to the atmosphere.

Economically, cost of construction of each system is determined as well as operating costs. Anticipated revenues are also listed.

INTRODUCTION

Because of the increasing value of raw and scrap materials and of energy, municipal solid waste recovery and incineration systems are becoming more feasible. Also, because of increasing interest in environmental protection and increasing land value, methods of solid waste disposal such as ocean-dumping or landfilling have become less and less attractive.

Recovery of materials such as those extracted by the process considered here (ferrous metal, glass, aluminum, and paper fiber) results in the conservation of natural resources, as well as a source of revenue to the community. Treatment and incineration of solid waste permits a reduction of approximately 95% by volume[1] of the solid material which must be disposed of by landfill. Heat resulting from the incineration can be used to generate steam which is typically used in the generation of electricity or for heating purposes. Stack gas can be cleaned using electrostatic precipitators; process water used in the solid waste recovery system can be recycled through a settling tank or other purification systems.

A major area of study covered in this report is the use of basically pure oxygen feed to the incinerator, compared with the traditional practice of air feed as the combustion medium. The use of oxygen feed permits the use of considerably more recycled product gas to control the combustion chamber temperature than is possible when using air. In this way, the amount of stack gas (with its wasted heat content) is approximately 43% by weight of the amount of stack gas which would have to be treated by the electrostatic precipitator before being exhausted to the atmosphere if air was used. Also, the amount of nitrogen oxide pollutants produced when using the oxygen feed is greatly reduced when compared with the amount produced by the traditional process.

Footnotes

1. Neff, N. Thomas, Solid Waste and Fiber Recovery Demonstration Plant for the City of Franklin, Ohio, U. S. Environmental Protection Agency Report No. EPA-SW-47D.I-72, National Technical Information Service, Springfield, Va., 1972, pg. 72.

General Information

In developing a solid waste recovery and incineration system, a base population of 500,000 people was chosen. Using projections listed in the literature,[1] it is estimated that by 1980 5.8 pounds of waste will be generated daily by each American citizen. Therefore, if the solid waste disposal system is to meet the needs of the base population for at least the next six years, it must be able to treat 2.9 million pounds daily (1,450 tons) of the waste.

A typical composition of municipal solid waste[2] is given below:

Component	Weight %	Pounds/Hour	Tons/Hour
Water	20.73	25,046	12.52
Carbon	28.00	33,833	16.92
Hydrogen	3.50	4,229	2.12
Oxygen	22.35	27,006	13.50
Nitrogen	0.33	399	0.20
Sulfur	0.16	193	0.10
Non-Combustibles	24.93	30,124	15.06
	Total	120,834	60.42

Having a specific volume of about 150 cubic feet/ton[3] (13.33 lb/ft^3), a storage pit for one day's supply of solid waste must hold 217,550 cubic feet or about 8060 cubic yards of material.

During the solid waste recovery process, the composition of the material is changed in the following ways:

1. 85% of the non-combustible material is removed (25,604 pounds/hour).
2. 21,750 pounds/hour of paper fiber is recovered. The paper

fiber is assumed to have a composition basically like cellulose of $(C_6H_{10}O_5)_n$ or 44.44% carbon, 6.18% hydrogen, and 49.38% oxygen. Therefore, 9665.7 pounds of carbon, 1344.15 pounds of hydrogen, and 10740.15 pounds of oxygen are removed from the solid waste each hour.

3. During the solid waste recovery process, water is added to make a slurry. Some of this water is removed before the waste is sent to the incinerator. However, 65,880 pounds of water per hour remain with the solid waste. Overall, 114,320 pounds of this material will be fed to the incinerator per hour.

Solid Waste Component	Pounds/Hour to Incinerator
Water	65,880
Carbon	24,167.3
Hydrogen	2,894.85
Oxygen	16,265.85
Nitrogen	399
Sulfur	193
Non-Combustibles	4,520

Thermal and chemical equilibriums within the incinerator were determined through the development of digital computer program GARBAGE. Corresponding to a pound of solid waste feed (excluding non-combustibles), the gram moles of each solid waste component within that pound are listed with fresh feed to the incinerator; this is in addition to the gas being used as the combustion medium. The values are listed in Appendix A.

The amounts of gas being added to the incinerator as fresh feed are chosen such that in combination with the recycled product gas, excess oxygen is near 5%. This is admittedly low, but because of the completely shredded nature of the waste, more oxygen was felt not to be necessary.

Type of Combustion Medium	Pounds/Hour of Fresh Gas to Incinerator
Air	Oxygen - 74,296.4
	Nitrogen - 258,005.8
Pure Oxygen	Oxygen - 74,296.4
	Nitrogen - 1,625.2

The pure oxygen feed was assumed to be at least 97.9% pure. Pure oxygen feed requirements are therefore 911 tons/day. Correspondence with Mr. P. G. Foust of Air Products and Chemicals, Inc. of Allentown, Pa. revealed that a 1000 ton/day facility would be suitable.

Temperatures in municipal solid waste incinerators should be at least 1200°F. to 1500°F. to completely eliminate odors.[4] For this reason and by comparison with present incinerators, recycle ratios of 0.1 for air feed and 0.6 for oxygen feed have been chosen where recycle ratio is defined as the ratio of moles of recycle gas to moles of fresh feed. Adiabatic flame temperatures are found to be about 2300°F. for the air system and 2270°F. for the pure oxygen system.

Eight major chemical reactions are expected to occur within the incinerator. They are:

1. $C + .5O_2 \rightarrow CO$
2. $CO + .5O_2 \rightarrow CO_2$
3. $.5N_2 + .5O_2 \rightarrow NO$
4. $NO + .5O_2 \rightarrow NO_2$
5. $H_2 + .5O_2 \rightarrow H_2O$

6. $S + O_2 \rightarrow SO_2$

7. $SO_2 + .5O_2 \rightarrow SO_3$

8. $H_2 + S \rightarrow H_2S$

The product gas composition for each of the processes being considered is listed below:

Chemical Species	Air System Weight %	Pure Oxygen System Weight %
H_2O	20.8	49.56
O_2	.01	2.52
N_2	58.53	1.1
CO_2	19.6	46.73
Others	1.06	.09

This indicates the presence of roughly ten times the amount of pollutants in the product gas from the air system as from the pure oxygen system.

Using results obtained from the computer program GARBAGE and scaling them up to the incinerator feed, the tables of flow rates on the following pages were obtained. To scale up, values from the computer program are multiplied by the number of pounds of combustible material fed into the incinerator per hour (109,800).

As can be seen from the data, total pound moles of stack gas for the air system is 2.25 times the total pound moles of stack gas for the pure oxygen system. Total pound moles of recycle gas for the air system is .324 times the total pound moles of recycle gas for the pure oxygen system. Also, total pound moles of product gas (stack gas and recycle gas) for the air system is 1.39 times the total pound moles of product gas from the pure oxygen system.

TABLE 1

Air System

Chemical Species	Pounds/Hour Fresh Feed	Pounds/Hour Recycled	Pounds/Hour Total Feed
H_2O	65,880	10,875.4	76,755.4
C	24,167.3	0	24,167.3
H_2	2,894.85	0	2,894.85
O_2	90,562.25	533.6	91,095.85
N_2	258,404.8	29,774.3	288,179.1
S	193	trace	193
non-combustibles	4,520	0	4,520
CO	0	.74	.74
CO_2	0	10,102.	10,102.
NO	0	15.2	15.2
NO_2	0	trace	trace
SO_2	0	.18	.18
SO_3	0	trace	trace
H_2S	0	trace	trace
Totals:	446,622.2	51,301.42	497,923.62

TABLE 2

Air System

Chemical Species	Pounds/Hour Purged	Pound Moles Recycled/Hour	Pound Moles Purged/Hour
H_2O	91,927.4	604.2	5,107.1
C	0	0	0
H_2	.2	0	.1
O_2	4,591.5	16.68	143.5
N_2	258,758.9	1,063.37	9,241.4
S	11.7	trace	.36
non-combustibles	4,520 as solid	0	-----
CO	6.13	.03	.22
CO_2	86,674.5	229.6	1,969.87
NO	131.3	.5	4.38
NO_2	.38	trace	.01
SO_2	.17	.003	.003
SO_3	.001	trace	trace
H_2S	.001	trace	trace
Totals:	446,622.2	1,914.383	16,466.943

TABLE 3

Pure Oxygen System

Chemical Species	Pounds/Hour Fresh Feed	Pounds/Hour Recycled	Pounds/Hour Total Feed
H_2O	65,880	73,952.38	139,832.38
C	24,167.3	0	24,167.3
H_2	2,894.85	0	2,894.85
O_2	90,562.25	3,789.46	94,351.71
N_2	2,024.2	1,691.72	3,715.92
S	193	4.1	197.1
non-combustibles	4,520	0	4,520
CO	0	2.39	2.39
CO_2	0	71,245.63	71,245.63
NO	0	9.42	9.42
NO_2	0	trace	trace
SO_2	0	trace	trace
SO_3	0	trace	trace
H_2S	0	131.47	131.47
Totals:	190,241.6	150,826.57	341,068.17

TABLE 4

Pure Oxygen System

Chemical Species	Pounds/Hour Purged	Pound Moles Recycled/Hour	Pound Moles Purged/Hour
H_2O	92,042.2	4,108.46	5,113.46
C	0	0	0
H_2	0	0	0
O_2	4,675.2	118.42	146.1
N_2	2,045.4	60.42	73.05
S	4.87	.13	.15
non-combustibles	4,520 as solid	0	-----
CO	2.97	.08	.11
CO_2	86,782.7	1,619.22	1,972.33
NO	10.95	.31	.36
NO_2	trace	trace	trace
SO_2	trace	trace	trace
SO_3	trace	trace	trace
H_2S	157.3	3.87	4.63
Totals:	190,241.6	5,910.91	7,310.19

Regarding the amount of heat released, the value obtained from the computer program is 4404.76 BTU per pound of combustible material or 4230.6 BTU per pound of waste entering the incinerator. Therefore, the total heat released within the incinerator is 483,642,192 BTU per hour. Heat calculations made in the computer program required the data listed on the following pages. Assuming that the boiler and power generating system obtains 40% efficiency, 56,624.6 kwh per hour of electricity are produced.

Stack gas is treated by an electrostatic precipitator to remove fly ash.

TABLE 5

Heat Capacity Data[5]

Where Mark Equals	Equation Form
+1	$C_p = A + BT + CT^2$
-1	$C_p = A + BT + C/T^2$

Chemical Species	A	B	C	Mark
C	4.03	.00114	-.204E+06	-1
O_2	6.15	.0031	-.923E-06	+1
CO	6.42	.00166	-.196E-06	+1
CO_2	6.21	.0104	-.354E-05	+1
N_2	6.83	.0009	-.120E+05	-1
NO	7.03	.00092	-.140E+05	-1
NO_2	10.1	.00228	-.167E+06	-1
H_2	6.52	.00078	.120E+05	-1
S	5.26	-.0001	.360E+05	-1
SO_2	11.0	.00188	-.184E+06	-1
SO_3	13.9	.0061	-.322E+06	-1
H_2S	6.66	.00513	-.854E-06	+1
H_2O	7.3	.00246	.0	-1

TABLE 6

Reaction No. (pages 6 and 7)	Heat of Reaction (cal/gram mole)	Equilibrium Data[6] Slope	Intercept
1.	-26,420	5980	4.6
2.	-67,640	14700	-4.6
3.	21,600	- 4690	.7
4.	-13,640	3385	-3.9
5.	-57,790	13000	-2.9
6.	-124,200	35600	1.4
7.	-23,450	11800	-11.4
8.	-58,020	2420	5.07

Footnotes

1. Niessen and Chansky, "The Nature of Refuse," Proceedings of 1970 National Incinerator Conference, The American Society of Mechanical Engineers, New York, 1970, pg. 16.

2. "Municipal Incineration," Bulletin D-61, M. H. Detrick Co.

3. Corey, Richard C., Principles and Practices of Incineration, Wiley-Interscience, New York, 1969, pg. 76.

4. Ibid., pg. 79.

5. a. Henley and Bieber, Chemical Engineering Calculations, McGraw-Hill Book Co., New York, 1959, pg. 412-428.

   b. Schmidt and List, Material and Energy Balances, Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1962, pg. 388-407.

   c. Smith and Van Ness, Introduction to Chemical Engineering Thermodynamics, McGraw-Hill Book Co., New York, 1959, pg. 122.

6. a. Balzhiser, Chemical Engineering Thermodynamics, Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1972, pg. 670.

   b. Smith and Van Ness, Introduction to Chemical Engineering Thermodynamics, McGraw-Hill Book Co., New York, 1959, pg. 423.

Solid Waste Recovery System

The solid waste recovery system is patterned after the process used at the Franklin, Ohio Solid Waste and Fiber Recovery Demonstration Plant.[1] This process was chosen because of its proven capability in recovering roughly 65% of the metal, 50% of the glass, and 45% of the paper fiber from the solid waste.

A flow chart and key are shown on the following pages. Solid lines between blocks represent the flow of solid waste and, at the incinerator, the flow of the combustion medium being used. Dashed lines represent the flow of major water streams.

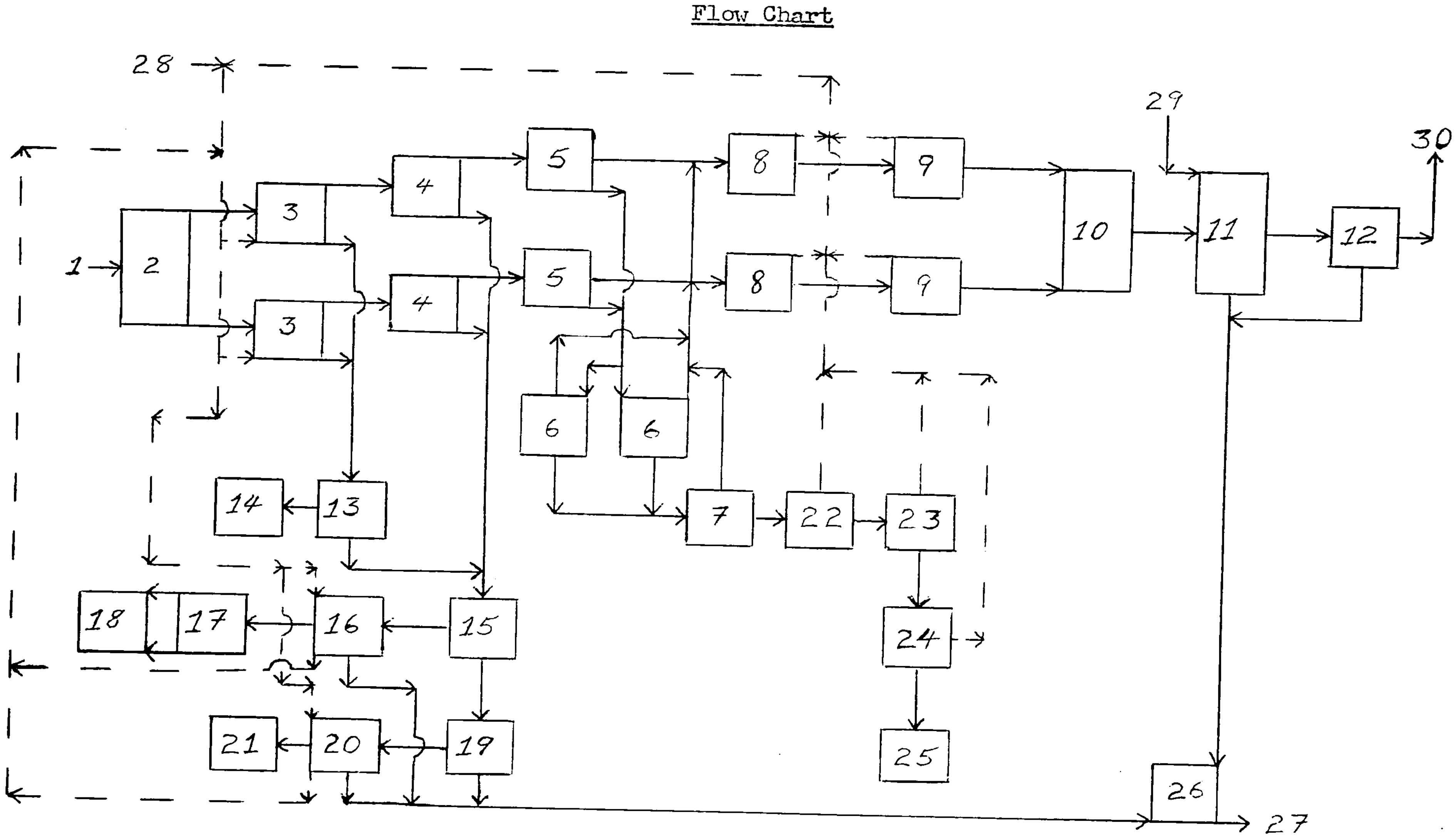
The process involves the shredding of the solid waste and the formation of a slurry, 96% by weight of water. Centrifugal action is used in both the pulping units and liquid cyclones to remove 85% of the non-combustibles. From these non-combustible streams, the ferrous metal, glass, and aluminum are extracted.

Ferrous metal is recovered by a magnetic drum and conveyor. Glass, smashed in the crusher unit through which the non-combustibles pass, is screened out, washed, and color-sorted by a Sortex unit. Aluminum is recovered using a zig-zag air classification column, and washed and screened to remove any adhering impurities. The remaining non-combustibles are disposed of in a landfill.

The slurry from the cyclones now enters the fiber recovery process. Twin Black Clawson VR Classifiner screening units with .125 inch diameter openings and twin Selectifier screening units

FIGURE 1

Flow Chart



KEY TO FLOW CHART

Unit Number	Unit Description
1	truck dumping port
2	solid waste storage pit
3	twin Hydrapulper shredder units
4	twin liquid cyclones
5	twin Classifiner screening units
6	twin Selectifier screening units
7	battery of three cyclone cleaners in series
8	twin Hydradenser units
9	twin cone presses
10	storage tank for burnable material
11	incinerator and boiler
12	electrostatic precipitator
13	magnetic separator
14	ferrous scrap container
15	glass recovery unit
16	glass washing and screening unit
17	clear and colored glass separator
18	glass scrap containers
19	aluminum recovery unit
20	aluminum washing unit
21	aluminum scrap container
22	Hydrasieve
23	Hydradenser unit
24	cone press

Unit Number	Unit Description
25	paper fiber container
26	non-combustibles dump
27	truck to landfill
28	fresh water added to recycled water
29	combustion medium (either air or oxygen)
30	cleaned stack gas

with .0625 inch diameter openings remove coarse impurities such as cloth and rubber from the paper fibers. Fine high density impurities such as particles of dirt and glass are removed by a battery of three centrifugal cleaners. The remaining paper fiber stream is further cleansed of organic fines as it passes over a Hydrasieve unit, manufactured by Combustion Engineering Company. Fines pass through the .020 inch slots of this unit while the paper fiber is drawn off the sieve. Dewatering of the paper to about 40% by weight of water is accomplished by a Black Clawson Hydradenser (an inclined screw thickener) and Rietz cone press. The water is recycled through a settling tank.

Impurities and fines removed from the paper fiber are returned to the twin streams of unrecoverable material. These streams are then dewatered by twin Black Clawson Hydradensers and Rietz cone presses to about 57.6% by weight of water and dumped into a storage tank capable of holding one day's supply of feed to the incinerator. Water removed by these units is also recycled through the settling tank.

The size of each of the twin process units will be about five times the sizes used in the demonstration plant which could conceivably handle 150 tons per 24 hour day. Therefore, the total size of the solid waste recovery plant being considered here may be about ten times the size of the Franklin, Ohio facility (not including the fluidized bed reactor/incinerator and the initial storage area) or about 1100 feet by 840 feet.

Hydrapulpers

Solid waste is loaded by crane into the feed hoppers of the twin Hydrapulper units, developed by Black Clawson Company. Each of the units accommodates 725 tons/day of municipal solid waste or 60,417 pounds per hour. The Hydrapulper is a hammermill shredder which converts the refuse into a slurry (96% by weight of water). The amount of water added to each Hydrapulper is 1,136,892 lb/hr or 136,281.3 gallons/hour.

A certain amount of non-pulpable material, 11% of the solid waste or 6,458 lb/hr from each pulper, is ejected by centrifugal force through a side channel around the base of each pulper. Some of the water added to the pulpers passes over this material to wash it. The slurry is extracted from the Hydrapulpers, 1,190,851 pounds per hour from each pulper, through the perforated bottom and pumped into the twin liquid cyclones.

Twin Liquid Cyclones

Approximately 10.5% of the solid waste or 6,344 lb/hr of the typically more dense non-combustible material is ejected from each cyclone. This material will be combined with the non-combustible material ejected by the Hydrapulpers after the latter material has been subjected to ferrous metal recovery. The remaining slurry from each cyclone, 1,184,507 lb/hr, passes to the Classifiner screening units. These numbers and those listed for the entire recovery system are based on data obtained at the demonstration plant.

Ferrous Metal Recovery

Of 12,916 lb/hr of material ejected from the Hydrapulper units, 8,700 lb/hr of ferrous metal is recovered by a magnetic drum and conveyor system of the type diagrammed on the next page. Electromagnets having a strength of 5,000 gauss should be sufficient for this purpose.[2] The ferrous metal recovered, summing to 104.4 tons per day, dumps into a shipping container. The remaining 4,216 lb/hr of non-combustibles is combined with the ejected stream of non-combustibles from the twin liquid cyclones. From this total stream of 16,904 lb/hr, glass and aluminum recovery is made.

Glass Recovery

The stream of non-combustibles enters a crusher unit which resembles a large piston. The brittle glass is crushed to a small size at this point. Much of the other non-combustibles is malleable and therefore, should only be deformed in this process. Glass and other fines are extracted by passing the stream over a screen with about .25 inch diameter openings. This extracted stream is washed and screened to remove adhering impurities and fines. The remaining glass is split into two streams, one of colored glass and one of clear glass by a Sortex separator of the type shown on the next page. The recovered glass, 42.768 tons per day of clear glass and 29.736 tons per day of colored glass, are dumped into shipping containers. These flow rates correspond to 3,564 lb/hr of clear glass and 2,478 lb/hr of colored glass.

FIGURE 2

Ferrous Metal Recovery

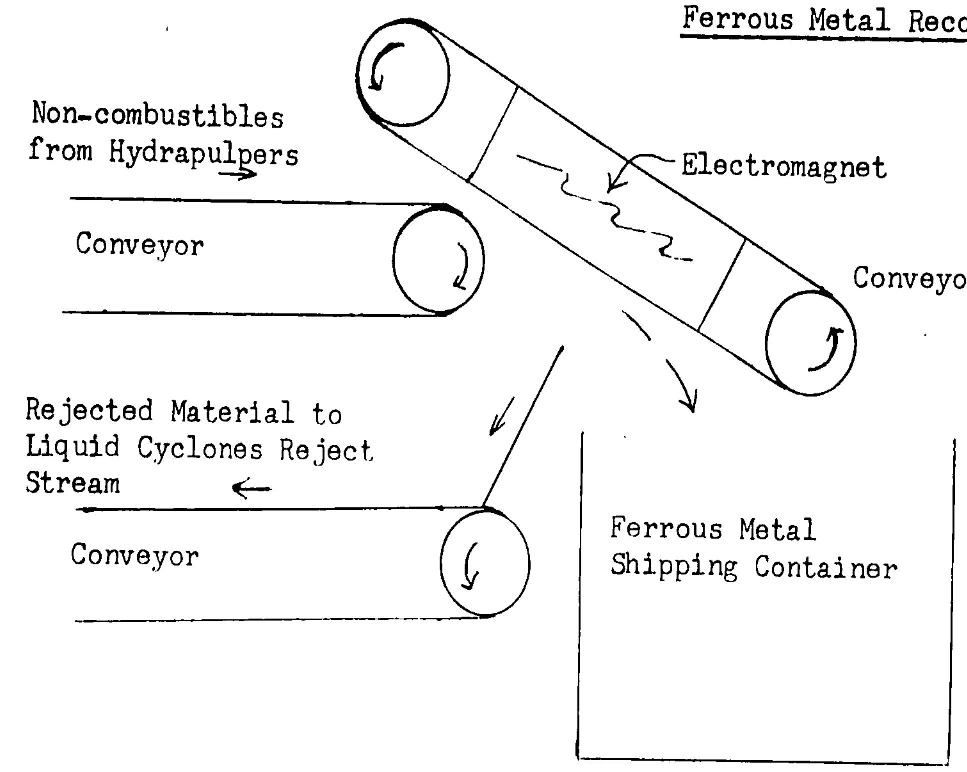
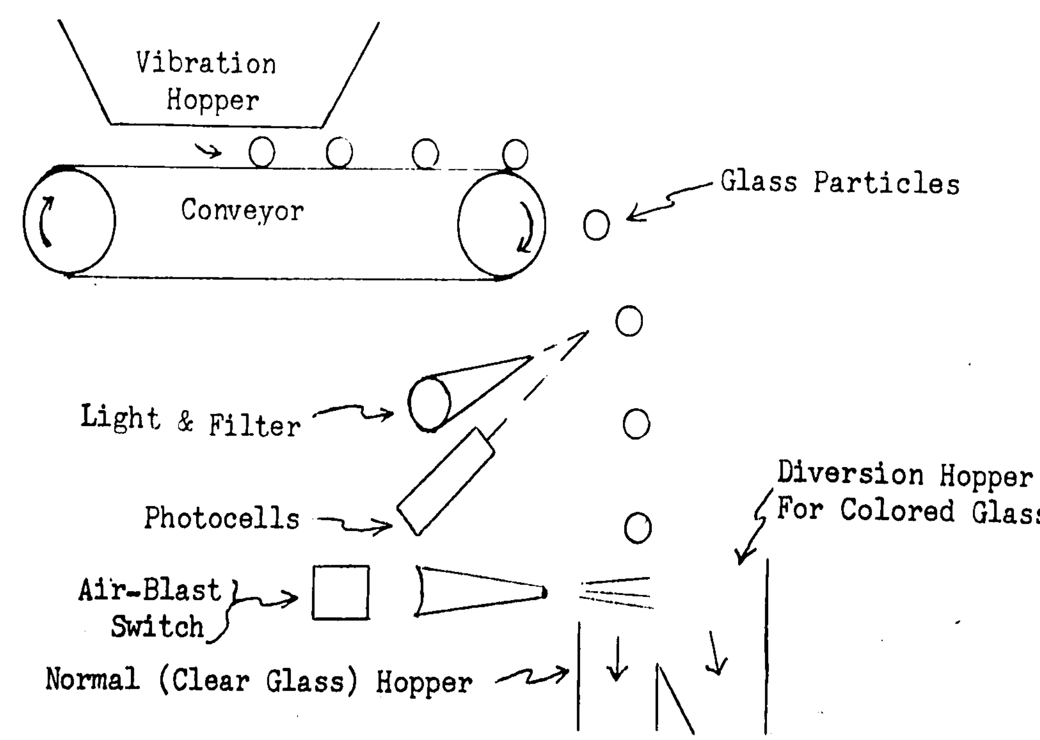


FIGURE 3

Sortex Glass Separator



Aluminum Recovery

From the remaining non-combustibles, 450 lb/hr of aluminum is recovered, washed, and screened to remove any adhering impurities. The recovery is accomplished using a zig-zag air classification column. A diagram of this device is shown on the following page. According to the Stanford Research Institute, an air velocity through the column of 2500 to 3000 feet per minute is required to separate metal, glass, and stone. It is anticipated that the aluminum will be drawn off the base of the column with low density impurities. For a list of densities of refuse components, see TABLE 7. The low density impurities are washed and screened off of the aluminum and 5.4 tons per day of aluminum are dumped into a shipping container. Removed impurities from the glass and aluminum recovery processes and the remaining non-combustibles, equal to 10,412 lb/hr, are disposed of in a landfill.

Classifiner Screening Units, Selectifier Screening Units

The remaining slurry from the liquid cyclones passes over twin Classifiner screening units as the first step in the recovery of paper fiber. 1,184,507 lb/hr of slurry is screened by each unit, the screens having .125 inch diameter openings. The long paper fibers are captured by the screen with some impurities. This stream then passes over twin Selectifier screening units to remove coarse impurities such as cloth and rubber, the screens having .0625 inch diameter openings. Impurities from both screening operations

FIGURE 4

Stanford Research Institute Zig-Zag Air Flow Classifier [3]

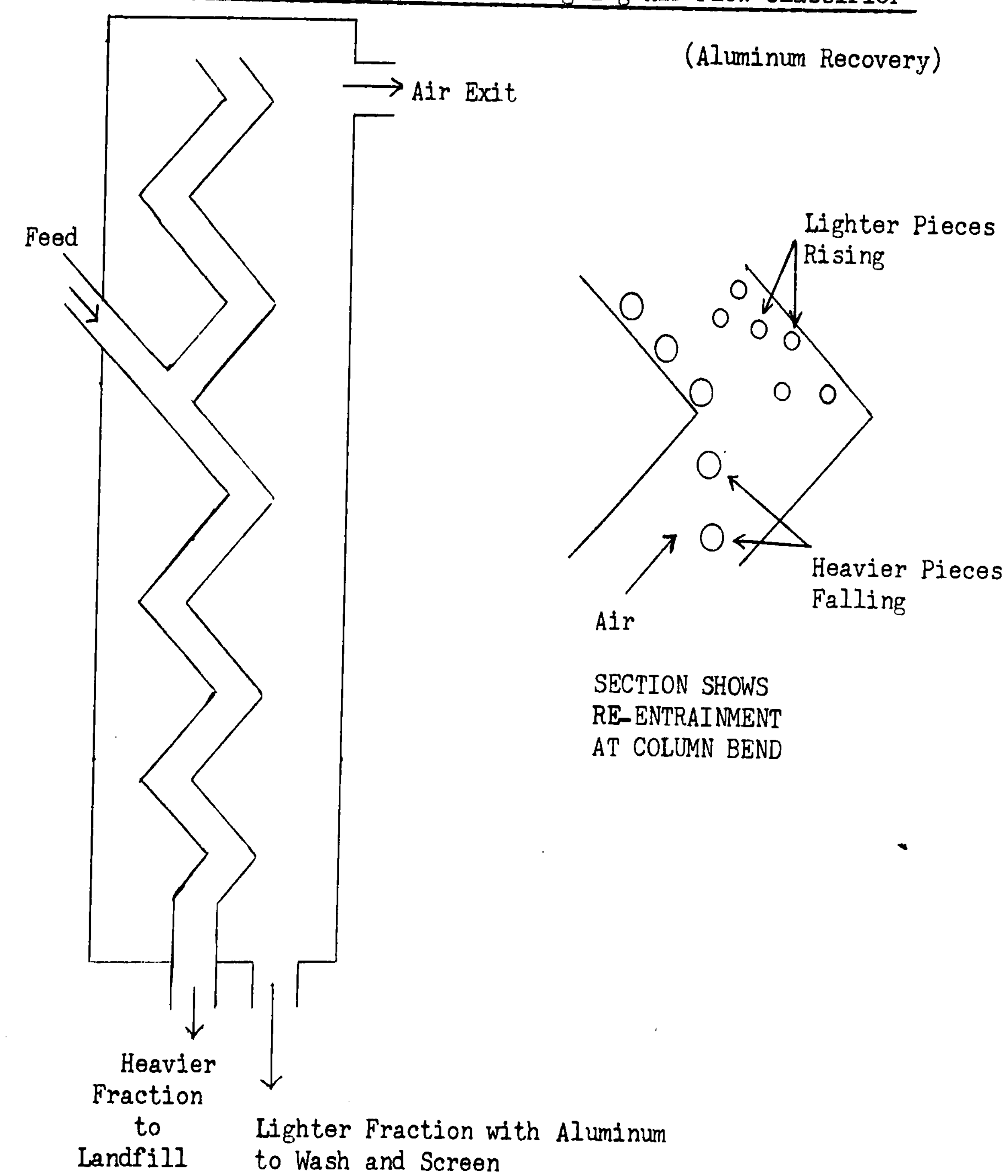


TABLE 7

Typical Densities of Refuse Constituents

Material	Density (lb/ft^3)
Lead	708
Copper	555
Nickel	537
Brass and Bronze	510 - 550
Iron	443 - 493
Zinc	412 - 450
Glass	162 - 187
Stone	140 - 175
Aluminum	168
Concrete	120 - 150
Brick	103 - 128
Magnesium	106 - 119
Plastics	50 - 125
Rubber	63 - 125
Dry Clay, Ash, Dirt	40 - 105
Cotton, Hemp	93
Leather	59
Paper	43 - 58
Wood	20 - 50
Food Waste	25 - 50
Yard Waste	20 - 30

are returned to the stream which will feed the incinerator. Basically, 367,398.5 lb/hr of wet paper fiber slurry is recovered from each set of Classifiner and Selectifier screening units, the slurry being 97% by weight of water due to the removal of the non-combustibles by the previous units. This wet paper fiber slurry is then fed to three centrifugal (cyclone) cleaners.

Cyclone Cleaners

These cleaning units are each fed one third of the total paper fiber slurry (734,797 lb/hr) or 244,923.3 lb/hr. This process removes any fine high density impurities as dirt and glass.

Hydrasieve

The remaining paper fiber slurry passes over this sieve with .020 inch slots. Organic fines are removed from the slurry and are combined with the impurities removed by the cyclone cleaners. These rejects are returned to the stream which will feed the incinerator.

Hydradenser, Cone Press

Hydradenser is an inclined screw thickener which removes 672,654.1 lb/hr of water from the wet paper fiber slurry. In other words, the slurry is reduced from 97% by weight of water to 65%. The remaining slurry of 62,142.9 lb/hr is fed into a Rietz cone press. The slurry is dewatered to 40% by weight of water, removing

25,892.9 lb/hr of water which is combined with the recovered water from the Hydradenser. This water, 698,547 lb/hr or 83,736.1 gal/hr, will be recycled through a settling tank. The remaining recovered paper fiber, 21,750 lb/hr of paper and 14,500 lb/hr of water, is dumped into a shipping container. Therefore, 261 tons/day of dry paper fiber are recovered.

Solid Waste Preparation for Incineration

Twin Hydradenser Units

These units, in preparing the remaining slurry of unrecovered material for incineration, will each process 817,108.5 lb/hr of slurry. Dewatering from 97% to 65% by weight of water is accomplished. Therefore, 748,004.5 lb/hr of water are removed by each unit, leaving 69,104 lb/hr for further processing.

Twin Cone Presses

The cone presses further dewater the streams from 65% to about 57.6% by weight of water, leaving 57,043.4 lb/hr from each press to be placed in the storage tank for future incineration. That is 32,857 lb/hr of water and 24,186.4 lb/hr of solid material from each press, which can be roughly expected and used for incinerator feed. 24,121.2 lb/hr of water are removed by the presses and added to the water removed by the twin Hydradenser units and the water removed from the recovered paper fiber. The total recovered water which is recycled through a settling tank and equals 2,218,677.2 lb/hr or 265,956.8 gal/hr. Recalling that 2,273,784 lb/hr or 272,562.6 gal/hr are required for the Hydrapulper units, total fresh water needed for this purpose is 55,106.8 lb/hr or 6,605.75 gal/hr.

Storage Tank

The storage tank for incinerator feed is designed to hold roughly one-day's supply of feed. Assuming that the feed has a density similar to water, a tank holding about 1850 cubic feet of the material should be sufficient.

Footnotes

1. Neff, N. Thomas, Solid Waste and Fiber Recovery Demonstration Plant for the City of Franklin, Ohio, U. S. Environmental Protection Agency Report No. EPA-SW-47D.I-72, National Technical Information Service, Springfield, Va., 1972.

2. Engdahl, R. B., Solid Waste Processing, U. S. Dept. of Health, Education, and Welfare, Washington, D. C., 1969.

3. Wilson, D. G., "Present and Future Possibilities of Reclamation from Solid Wastes," New Directions in Solid Waste Processing 1970, Technical Guidance Center for Industrial Environmental Control, University of Massachusetts, Amherst, Mass., 1970, pg. 18.

Incinerator

The incinerator chosen for this project is similar to the Chicago Northwest Incinerator using a grate-stoker designed by IBW-Martin. However, where the Chicago Northwest Incinerator was designed to produce steam for heating purposes in the local area, the use of steam for generating electricity has been considered here. This requires much higher steam pressure and temperature such as 3500 psig. and 1000°F. to provide efficient power generation.[1] Assuming that the efficiency of the power generation system is 40%, the total energy recovered is 193,316,547 BTU/hr or 56,624.6 kwh of electricity.

The required volume of the incinerator chamber can be estimated using the following equation:[2]

$V_c = (BF)/I$

where: V_c = chamber volume = cubic feet

B = heating value of fuel = BTU/lb

F = firing rate = lb/hr

I = combustion intensity = BTU/ft^3-hr-atm

For the type of refuse being considered here, I = 13750 BTU/ft^3-hr-atm can be assumed. Therefore, a chamber volume of at least 35,174 ft^3 is required, regardless of whether air or pure oxygen feed is used. In other words, the incinerator volume is independent of the combustion medium used. Roughly the same amount of steam tubing will be required because of the low heat transfer coefficient of the product gas. Therefore, an incinerator chamber of approximate length = 35 feet, width = 20 feet, and height = 50 feet can be anticipated.

Because of the low level of noxious gases produced from both the air and pure oxygen systems, it is felt that only an electrostatic precipitator to remove fly ash will be necessary to treat the stack gas. (Experience in the field may indicate the need for venturi scrubbers.) The air system will require a precipitator of about 2.25 times the capacity of the precipitator for the pure oxygen system. Assuming the purge stream enters the precipitator at 500^{o}F., approximately 12,337,320 ft.^{3}/hr. or 205,622 cfm. of gas must be treated for the air system. For the pure oxygen system, about 5,476,920 ft.^{3}/hr. or 91,282 cfm. of gas must be treated.

Fly ash and non-combustibles (roughly 4,520 lb/hr) are combined with the unrecovered non-combustibles extracted in the solid waste recovery system (about 10,412 lb/hr). This highly dense stream of fused and heavy non-combustibles, 14,932 lb/hr, is disposed of in a landfill.

It should be noted that the assumption was made in computer program GARBAGE that recycle streams entered the incinerator at the same temperature as the solid waste feed, 80^{o}F. That assumption greatly simplified the heat calculations. In an actual incinerator, recycle gas can be typically around 500^{o}F.

To consider the effects of the additional heat within the incinerator, average heat capacities in this temperature range for the recycle gas streams are .287 BTU/lb °F. for the air system and .333 BTU/lb °F. for the pure oxygen system. Accounting for the temperature difference between 500°F. and 80°F. and the heat of vaporization of water, 16,736,274 BTU/hr are added to the air system. The total feed, having an average heat capacity of .339 BTU/lb °F. would be raised about 100°F. higher to 2400°F. This is not enough to effect the reaction extents.

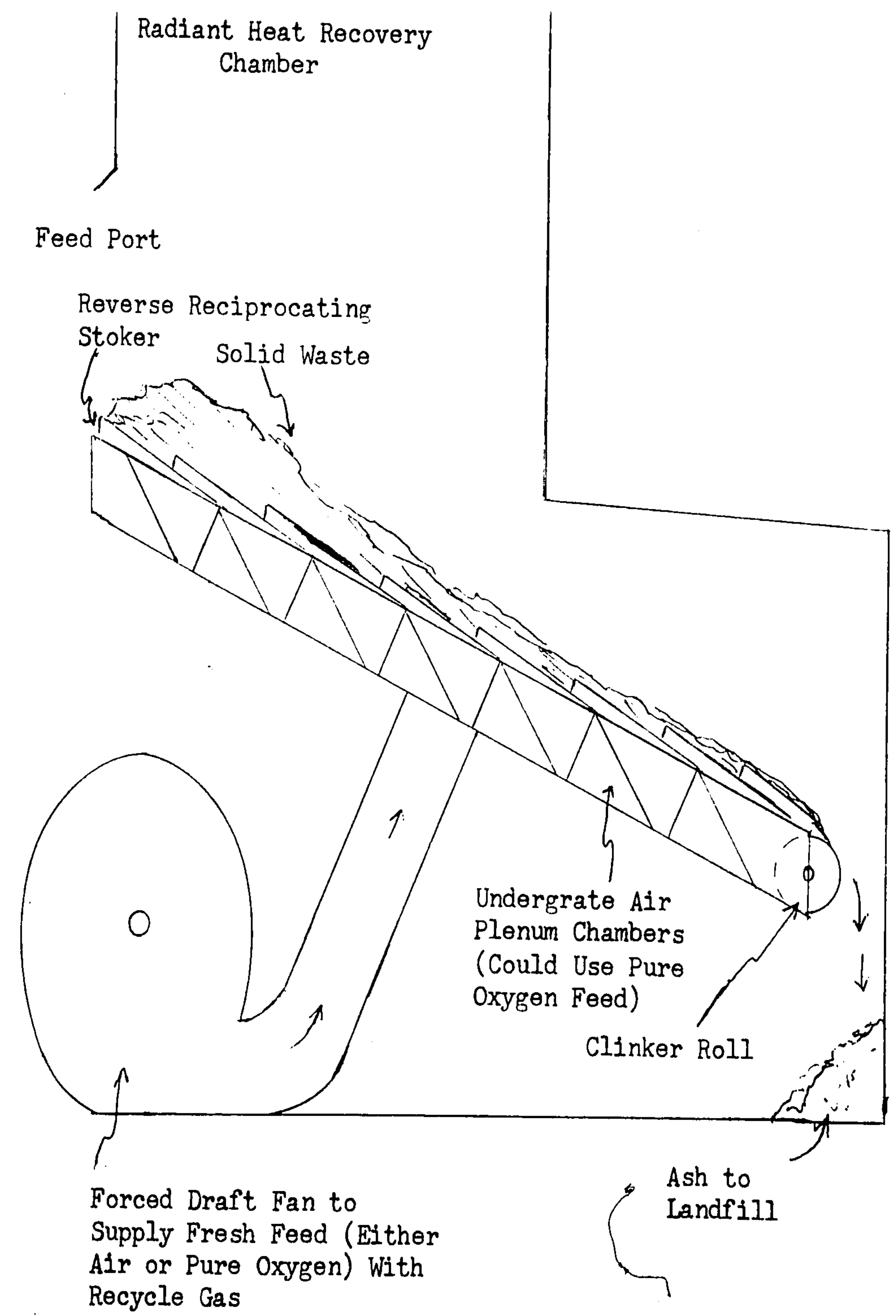
The effect of this additional heat for the oxygen system is greater because of the much larger amount of recycle gas. 92,850,598 BTU/hr are added to the system. This would raise the temperature of the total feed with an average heat capacity of .428 BTU/lb °F. to about 2905°F. from the 2270°F. temperature determined by the computer program. However, experience with the computer program indicates that this would only slightly effect reaction extents. (Temperatures above about 3500°F. have a stronger effect on the extents.) For the oxygen system, more recycle gas would be required to lower the temperature to about 2400°F., making total gas flow within the incinerator more similar to the air system's total gas flow. This all indicates that operating costs using either air or pure oxygen feed to the incinerator would be roughly the same for the incineration process.

Grate-Stoker

A diagram of the incinerator with the grate-stoker is shown on the next page. Used at Chicago's Northwest Incinerator and elsewhere,

FIGURE 5

Grate-Stoker Incinerator



the IBW-Martin grate-stoker has been successfully applied.[3] Reciprocating grate steps push burning refuse under fresh refuse to encourage complete incineration. The grate is inclined on a 26° angle, taking advantage of gravity in keeping the flow of fuel steady.

With Air Feed

Flow rates listed in TABLES 1 and 2 apply to the traditional air system. Because of the large amounts of fresh nitrogen fed into the system, only low recycle ratios are permitted and a large purge stream is necessary. The air is fed to the grate-stoker and flows up through the burning refuse to promote complete combustion.

With Pure Oxygen Feed

Flow rates listed in TABLES 3 and 4 pertain to the pure oxygen system. A much greater amount of recycle gas is needed to control the combustion chamber temperature. The purge stream is less than half of the amount obtained from an incinerator using the air system, resulting in a savings on electrostatic precipitator capacity. However, the 1000 tons/day, pure oxygen plant is costly and requires a significant level of maintenance. The plant can be expected to have a 5% downtime,[4] suggesting that a cryogenic storage tank would also be necessary to insure a steady flow of fresh combustion medium. The oxygen plant site would be 300 feet by 500 feet. A power requirement of 1350 kwh must be met.

Footnotes

1. Steam/Its Generation and Use, Babcock and Wilcox, New York, 1972, pg. 2-15.

2. Essenhigh, "Burning Rates in Incinerators," Proceedings of 1968 National Incinerator Conference, The American Society of Mechanical Engineers, New York, 1968, pg. 87.

3. Martin Refuse Incineration Plants, IBW-Martin Incinerator Group, Subsidiary of Ovitron Corp., E. Stroudsburg, Pa.

4. Correspondence with Mr. P. G. Foust, Air Products and Chemicals, Inc., Allentown, Pa.

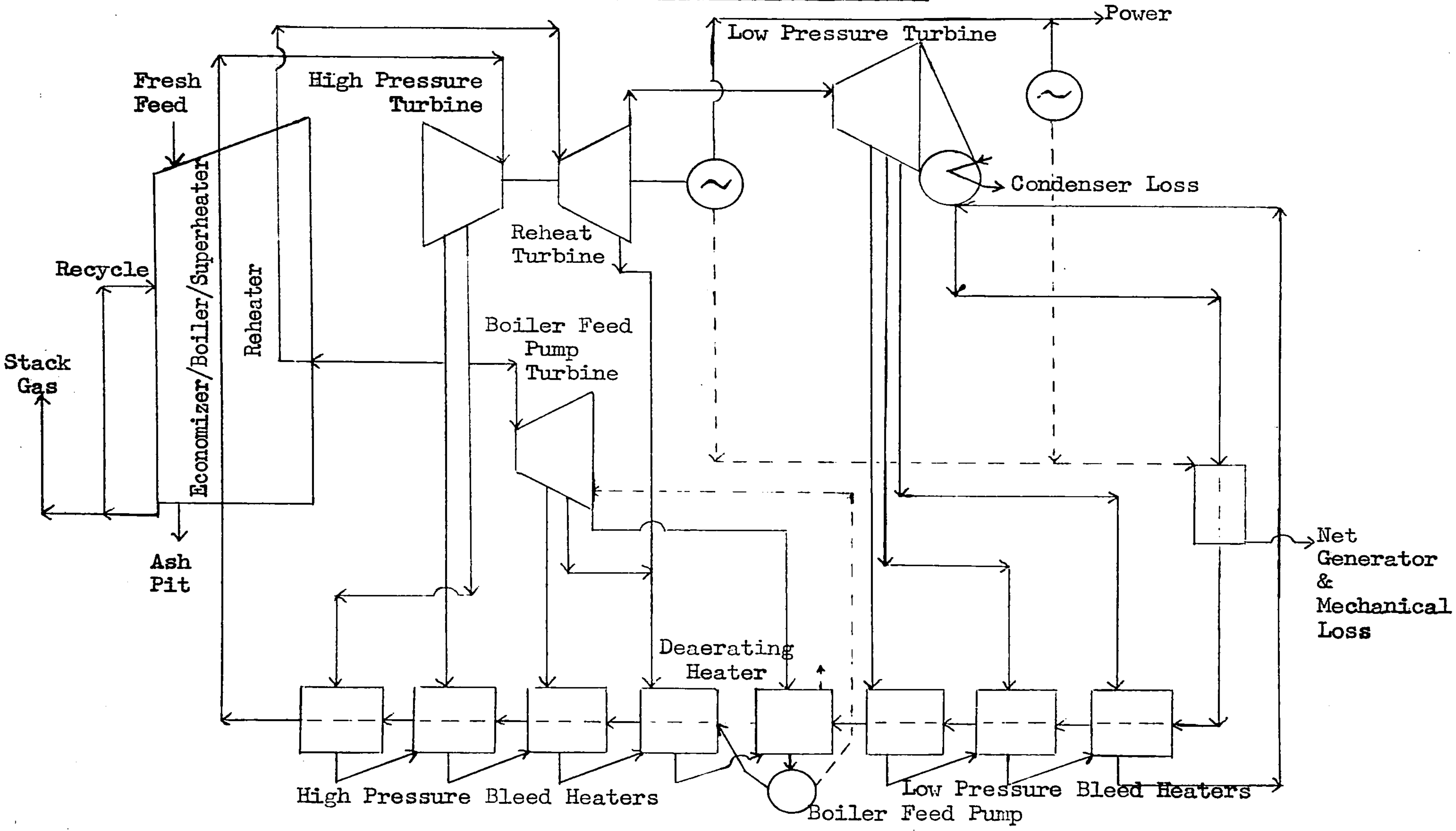
Electrical Generation

The generation of 56,624.6 kwh of electricity for each hour of incinerator operation is accomplished using a regenerative Rankine steam cycle. On Figure 6, the steam flow through the various process units is shown.[1] Steam at 3500 psig and 1000°F. is generated in the combustion chamber. Using a system of turbines, the electricity is produced. Figure 7 shows the steam cycle on a temperature versus entropy diagram. Total electrical generation per day is approximately 1,358,990 kwh.

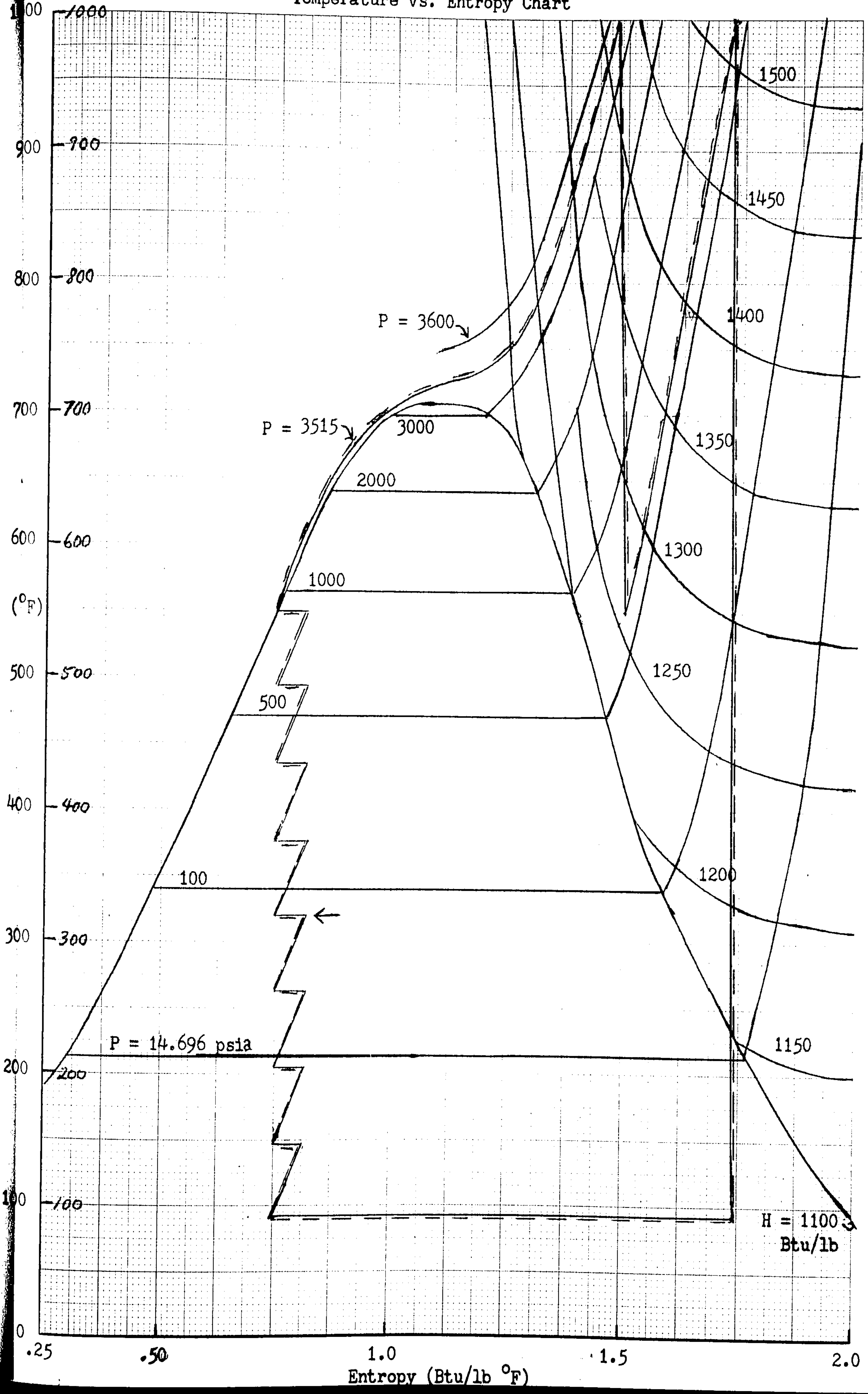
Footnotes

1. Steam/Its Generation and Use, Babcock and Wilcox, New York, 1972, pg. 2-15.

FIGURE 6
Regenerative Rankine Steam Cycle



STEAM **FIGURE 7**
Temperature vs. Entropy Chart



Economic Evaluation

Construction Costs

1. Land Estimate - includes initial storage pit, solid waste recovery system, incinerator, power generator system, electrostatic precipitator, and stack

   $= 1600 \text{ ft by } 840 \text{ ft} = 1.344 \times 10^6 \text{ ft}^2$

   With Oxygen Plant (300 ft by 500 ft) $= 1.494 \times 10^6 \text{ ft}^2$

   At \$45,000/acre,[1] air system land cost = \$1,378,100

   oxygen system land cost = \$1,543,388

   Using December of 1973 economic indices[2] and available data,[3] the following construction costs were determined:

2. Truck ports - includes tipping floor, scales, and accessories

   (\$373/ton-day in 1971[4]) x 1.174 = \$437.9/ton-day Dec. 1973

   or \$634,955

3. Storage pit - includes cranes, hoppers, and accessories

   (\$840/ton-day in 1971[5]) x 1.174 = \$986.16/ton-day Dec. 1973

   or \$1,429,932

4. Structure cost for solid waste recovery system

   (\$12.50/ft^2 in 1971[6]) x 1.185 = \$14.81/ft^2

   or \$924,000

5. Hydrasposal system[7] - includes Hydrapulpers, liquid cyclones, ferrous metal recovery, glass recovery, aluminum recovery, twin Hydradensers, twin cone presses, incinerator feed storage tank, and recycled water settling tank.

   Comparison of projected data in the literature for 500 ton/day and 150 ton/day plants with regard to dollar ratio over capacity ratio resulted in .682 of the projection ratio based solely on capacity. Using the process machinery economic index to obtain updating factor 1.034,[8] the following is obtained:

$3,110,000 for 500 ton/day 1972 system x 1.034 = $3,215,740

Therefore, $3,215,740 x 1450/500 x .682 = $6,360,090

6. Fibreclaim system[9] - includes Classifiner and Selectifier screening units, cyclone cleaners, Hydrasieve, Hydradenser, and cone press.

As was done for the Hydrasposal system, a similar comparison of dollar ratio to capacity ratio was made for the 500 ton/day and 150 ton/day plants. The result was 1.081 of what the projection ratio based solely on capacity equaled. Using the process machinery economic index of 1.034:

$2,700,000 for 500 ton/day 1972 system x 1.034 = $2,791,800

Therefore, $2,791,800 x 1450/500 x 1.081 = $8,752,014

7. Incinerator/Boiler/Power Generating system/Electrostatic Precipitator - waterwall incinerator construction

$3,364/ton for 300 ton/day 1970 system[10] x 1.193 = $4,014/ton
Plant Cost Index

$4,014 x 1372 ton/day to incinerator = $5,507,646.8

In order to more thoroughly compare electrostatic precipitator costs, data was used to determine the dollars/cfm treated.[11] The electrostatic precipitator for the air system would cost roughly $1.4/cfm treated (assuming 99% cleaning efficiency) or $287,870.8. The electrostatic precipitator for the pure oxygen system would cost roughly $1.6/cfm treated (assuming 99% cleaning efficiency) or $146,051.2. The difference between the two cost estimates is subtracted from the $5.5 million figure to obtain the total incinerator/boiler/power generating system/electrostatic precipitator cost estimate for the pure oxygen system or $5,365,827.2.

8. Oxygen Plant[12] - $6,500,000

Totals

	Air System	Pure Oxygen System	
Land	$1,378,100	$1,543,388	
Truck Ports	634,955	634,955	
Storage Pit	1,429,932	1,429,932	
Structure	924,000	924,000	
Hydrasposal	6,360,090	6,360,090	
Fibreclaim	8,752,014	8,752,014	
Incinerator/ Boiler/ Generation System/ Electrostatic Precipitator	5,507,646.8	5,365,827.2	
		6,500,000	Oxygen Plant
Totals:	$24,986,737.8	$31,510,206.2	

Operating Costs

Operating costs for the air system and the pure oxygen system would be roughly the same except for the following items.

1. Electrostatic Precipitator Operation[13] - For the air system, roughly $0.21/cfm/yr assuming 99% effectiveness or $43,180.6/yr. is required. For the pure oxygen system, roughly $0.26/cfm/yr assuming 99% effectiveness or $23,733.3/yr. is required.

2. **Oxygen Plant Operating Costs**[14] **- annual major costs**

Chems and Lubes	$8,000
Labor (8 men)	$120,000
Maintenance	$130,000
Power (at 1¢/kwh)	$118,260
	$376,260

Therefore, above the common operating costs to both air and pure oxygen systems, $43,180.6/yr. must be added to the air system operating cost while $399,993.3/yr. must be added to the pure oxygen system operating cost. Operating expenses per year will be $356,812.7 higher for the pure oxygen system than for the air system.

A list of anticipated revenues, common to either system being considered, follows:

Material	Rate	Annual Revenue
Ferrous Metal	$13.27/ton[15]	$505,666.6
Glass	$5/ton	132,319.8
Aluminum	$200/ton	394,200
Paper Fiber	$25/ton	2,381,625
Total for Recovered Material		$3,413,811.4
Electricity	$.01/kwh	4,960,313.5
Total Annual Revenues		$8,374,124.9

In order to examine the costs involved per ton processed, a complete list of annual operating expenses is shown on the following page:

Process	Unit Process Cost	Annual Operating Cost Air System	Oxygen System
Hydrasposal	\$7.78/ton[16]	\$4,117,565	\$4,117,565
Fibreclaim	\$3.34/ton	1,767,695	1,767,695
Incinerator/ Boiler/ Generating System/ Electrostatic Precipitator	\$1.13/ton[17]	565,881.4	546,434.1
Oxygen Plant			376,260
Total Operating Expenses		6,451,141.4	6,807,954.1
Total Revenues		8,374,124.9	8,374,124.9
Net Profit		1,922,983.5	1,566,170.8
Net Profit/Ton		\$3.63	\$2.96

This indicates the success which is possible when using efficient solid waste recovery. However, there is little stimulation for using the pure oxygen process (other than reduced pollution).

It should be noted that refuse transportation costs to the incinerator/recovery system are significant and would have to be provided for.

Footnotes

1.,6. Berkowitz, Solid Waste Separator Interim Progress Report, Franklin Institute Research Laboratories, Phila., Pa., 1972.

2.,8. Chemical Engineering, Vol. 81, No. 10, McGraw-Hill Book Co., New York, 1974.

3.,7., 9.,15., 16. Neff, N. Thomas, Solid Waste and Fiber Recovery Demonstration Plant for the City of Franklin, Ohio, U. S. Environmental Protection Agency Report No. EPA-SW-47D.I-72, National Technical Information Service, Springfield, Va., 1972.

4.,5. Warner, A., Plastics Solid Waste Disposal by Incineration or Landfill, Manufacturing Chemists Assoc., Washington, D. C., 1971.

10.,17. Fife, "Design of the Northwest Incinerator for the City of Chicago," Proceedings of 1970 National Incinerator Conference, The American Society of Mechanical Engineers, New York, 1970.

11.,13. Vandegrift, Shannon, and Gorman, "Controlling Fine Particles," Chemical Engineering, Vol. 80, No. 14, McGraw-Hill Book Co., New York, 1973.

12.,14. Correspondence with Mr. P. G. Foust, Air Products and Chemicals, Inc., Allentown, Pa.

Summary and Conclusions

Solid waste recovery is becoming more and more profitable due to the rise in the value of raw materials, such as ferrous metal, glass, aluminum, and paper fiber. A similar increase in the value of energy provides stimulation for solid waste incineration or pyrolysis, rather than landfill disposal. Analysis of comparative solid waste recovery and incineration systems using either air or pure oxygen as combustion mediums has shown that the use of pure oxygen offers no economic benefit and, in fact, is significantly more expensive. While the purge stream and level of pollutants are significantly reduced when using the pure oxygen system, the level of pollutants from the traditional air system is also low. Because of the temperature control and low heat transfer coefficients of the product gas, incinerator and boiler size for either system being considered will be about the same. Therefore, a pure oxygen system is not justified.

The use of solid waste as auxiliary fuel in a power generation station, as is done in St. Louis, or in the production of methanol through pyrolysis may prove to be more viable solutions to the solid waste disposal problem. The recently patented pyrolysis process,[1] developed at Union Carbide, results in the production of methanol which can be turned into methane. As natural gas becomes more scarce, this source of synthetic gas may be highly attractive.

Where incineration is planned, the effective use of solid waste recovery and of power generation can greatly improve the economic viability of a municipal solid waste disposal system.

Footnotes

1. Anderson, J. E., Solid Refuse Disposal Process and Apparatus, patent no. 3,729,298, April 24, 1973.

Appendix A

DESCRIPTION AND LISTING OF DIGITAL COMPUTER PROGRAM

Program GARBAGE accomplishes the calculation of the thermal and chemical equilibrium attained in a typical municipal incinerator. This is achieved through three trial-and-error solutions for a particular feed and recycle ratio and an initially assumed combustion temperature:

1. Calculation by subprogram BSOLVE of the extents of each of the chemical reactions involved is reiterated until equilibrium constants calculated using gas mole fractions match equilibrium constants obtained for each reaction from the literature.
2. Calculation of the recycle composition for a trial is made and values are compared with the recycle composition values of the previous trial. If the values for each of the components is the same for both trials, the computer proceeds to the third trial-and-error section. If the values are not the same within 0.1 of a gram mole, the latest determined recycle composition values are used in the revision of the total feed for which trial-and-error section #1 must again be satisfied. After trial-and-error sections #1 and #2 have been satisfied:
3. Calculation of the heat required to raise the reaction products

from ambient to the assumed combustion temperature is made and compared with the calculated total heat of reaction in order to determine the adiabatic flame temperature of the system. The combustion temperature is revised if necessary to within 10°F. of the combustion temperature possible. If a temperature revision is necessary, trial-and-error sections #1, #2, and #3 must again be individually satisfied.

When all three solutions have been made, volumetric flow rates, computed at standard temperature and pressure, and gram mole amounts of each chemical species in the purge and recycle streams are listed.

INDEX OF IMPORTANT VARIABLE NAMES

DATA REQUIRED:

Variable Name	Description
NS	number of chemical species
NR	number of chemical reactions + 1
NAME(J)	names given each chemical species
ALPHA(J) BETA(J) GAMMA(J)	heat capacity equation coefficients
MARK(J)	defines which form of heat capacity equation to use
NSOL(J)	identifies chemical species which maintain a solid state throughout combustion
NPR(J)	identifies chemical species which appear only as reactants from those which appear both as reactants and products of the reactions under study
STOIC(I,J)	stoichiometric coefficient of each chemical species in each reaction
STOIC(NR,J)	initial number of gram moles of each species
SLOPE(J) YINTCP(J)	literature values for each chemical reaction being considered, used in determining the equilibrium constant at the combustion temperature
HEAT(J)	heat of reaction in calories/gram mole for each reaction being considered

Two other values which must be inserted in the body of the program are:

RECYCLE	recycle ratio under consideration, defined as the ratio of gram moles of recycle gas to gram moles of fresh feed

TGUESSF(JN)	estimated combustion chamber temperature (adiabatic flame temperature)

It has also been necessary to stipulate that the chemical reaction $C + .5O_2 \rightarrow CO$ must be listed as the first reaction. Because of the heat of vaporization of water which must be considered in calculating the heat required to raise the reaction products to the combustion temperature, it is established that water be the last chemical species listed in the data. HVAP = 9700 calories/gram mole appears within the body of the program for the calculation described above.

OTHER IMPORTANT VARIABLES:

Variable Name	Description
NREACT	number of chemical reactions
B(J)	extent of each chemical reaction at the combustion temperature
BMIN(J),BMAX(J)	minimum and maximum extents, respectively, for which a reaction can proceed based on the amounts of each chemical species present
SENS2(J)	average heat capacity of each chemical species
VOL(J)	ideal gas volume of each species in cubic feet at TGUESSF(JN) after reaction
VOLSTP(J)	ideal gas volume of each species in cubic feet at standard temperature and pressure after reaction
XN(J)	final gram moles of each species after reaction
BMI(J),BMA(J),BOX(J)	values used in determining BMIN(J) and BMAX(J)
FEED(J)	gram moles of each species in the fresh feed
DELMOL(J)	difference between the total initial gram moles of each species and the final gram moles

GAS(J)	mole fraction of each gaseous species in the reaction product stream
SPURGE(J)	gram moles of each species in the purge stream
RECY(J)	gram moles of each species to be recycled
RECYL(J)	total gram moles of each species entering the reaction system
XXN(I,J)	RECYL(J) for each species for each trial in gram moles
TSPVOL(J)	ideal gas volume in cubic feet of each species in the purge stream at standard temperature and pressure
SU	total ideal gas volume in cubic feet of the purge stream at standard temperature and pressure
TREVOL(J)	ideal gas volume in cubic feet of each species in the recycle stream at standard temperature and pressure
SUU	total ideal gas volume in cubic feet of the recycle stream at standard temperature and pressure
TNSUM	gram moles of reaction product gas available
REC	gram moles of reaction product gas to be recycled
PURGE	gram moles of reaction product gas to be purged
AMAKEUP	gram moles of reaction product gas not present, but dictated for by an arbitrarily set, impossibly high recycle ratio
TGUESS	TGUESSF(JN) in degrees Centigrade
TREF	reference, ambient feed temperature = 298°C.
SUM4	total heat of reaction in calories
SUM5	total heat in calories necessary to raise the temperature of the reaction products to TGUESSF(JN)

The following list of variables and descriptions accompany subprogram BSOLVE, written by Dr. W. E. Ball of Washington University:

Variable Name	Description
KK	number of unknowns
B(J)	vector of unknowns (KK long), extents of each chemical reaction in this case
NN	number of equations - must be greater than or equal to KK
Z(J)	vector of computed values (NN long), want Z(J) = Y(J) in the output
Y(J)	vector of given values (NN long), mole fractions in this case
PH	function value equal to the sum of the quantities Z(J) - Y(J) squared, serving as a measure of the error
FNU	NU factor (set to 10.0 if originally set at 0.)
FLA	LAMBDA factor (set to .01 if originally set at 0.)
TAU	TAU factor (set to .001 if originally set at 0.)
EPS	EPSILON factor (set to .00002 if originally set at 0.)
PHMIN	cut-off point for recalculating Jacobian matrix, usually set to 0.
I	iteration count, initially must be 0
ICON	number of unknowns not satisfying the convergence requirement of: ABS(DELTA B(J))/(ABS(DELTA B(J)) + TAU).LE.EPS = 0 answer found =-1 no function improvement possible =-2 more unknowns than functions =-3 total variables are zero =-4 corrections satisfy convergence requirements but FLA is still large
FV	dummy variable vector passed on to FUNC and DERIV
DV	dummy variable vector passed on to DERIV

Variable Name	Description
BV(J)	code for variable type (KK long) = 0. B(J) is not variable = 1. B(J) is variable and numerical derivatives are to be used; used in this case =-1. B(J) is variable and analytical derivatives are to be used
P(J)	Jacobian vector arranged columnwise NN by KK, vector is NN*KK long P(L) = DZ(I)/DB(J) with L = I + (J-1)*NN Total vector length is KK*(NN + 2) + NN. Locations starting with NN*KK + 1 used for scratch. Note this vector is calculated by DERIV if any BV(J) = -1.
FUNC	name of function subprogram to be written by user - name must appear in external statement in main program - this routine must always be supplied (this is subprogram FNTX in this case) CALL FUNC(KK,B,NN,Z,FV) - these variables are as previously defined
DERIV (not used here)	name of subprogram used to evaluate derivatives if indicated by BV(J). The name of the subprogram must appear in the calling program as an external statement. CALL DERIV(KK,B,NN,Z,PJ,FV,DV,J,JTEST) Z(J) = vector (NN long) of values of the equations - need not be calculated in unless JTEST = -1 returned PJ(J)= the vector of derivatives (NN long) calculated by the subprogram - this is the Jth column of the Jacobian J = the index of the variable for which derivatives are to be calculated by DERIV JTEST= if the derivatives have been calculated, set JTEST to zero. If a value of -1 is returned, BSOLVE will attempt to take numerical derivatives based on the Z vector returned.
KD	the number of rows of the storage matrices A and AC in the calling program; KD must be greater than or equal to KK
A,AC	scratch matrices of dimension KD by (KK + 2)
GAMM	the angle in degrees between the modified Newton-Raphson direction and the steepest descent direction - output

A thorough mathematical explanation of the method used in BSOLVE for solution of the extents of each chemical reaction is given in the literature.[1] Regarding BSOLVE, difficulty in obtaining a satisfactory solution was initially encountered. This problem was eliminated by having BMIN(J) and BMAX(J) specifically computed for each reaction. (This was not shown to be necessary by the literature source.[2]) Correspondence with Mr. Edward M. Rosen, Manager of Systems Technology for Monsanto Company, revealed another method[3] of resolving the problem encountered. It is described below.

Set up additional equations of the type:

$$n_i = n_{io} + e\alpha_i \qquad (1)$$

for each component. With each equation added, one adds an additional unknown n_i. In doing this, hard bounds can be placed on each e_i and n_i:

$$0 \leq n_i \leq \text{large number}$$

$$\text{negative large number} \leq e_i \leq \text{large number} \qquad (2)$$

Linear constraints of equation (1) are no longer present and this formulation can be handled by BSOLVE. In the case used for this report, an equation would have been written for each chemical species along with those written for extents of each reaction. Each equation would have the hard bounds shown in equation (2).

A listing of the entire computer program along with the outputs used in designing the incinerator systems, for air and for pure oxygen feeds respectively, follows.

HHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHHH


```
      PROGRAM GARBAGE (INPUT, OUTPUT)
      EXTERNAL FNTX
C  NS IS THE NUMBER OF CHEMICAL SPECIES.
C  NREACT IS THE NUMBER OF REACTIONS.
C  THE REACTION OF C + 1/2 O2 FORMING CO MUST APPEAR AS THE FIRST RXN.
C   IN ACCOUNTING FOR LATENT HEAT OF VAPORIZATION OF WATER, IT HAS BEEN
C   NECESSARY TO STIPULATE THAT THE LAST CHEMICAL SPECIES MUST BE WATER.
C   YOU MUST HAVE WATER AS THE LAST CHEMICAL SPECIES OR CHANGE HVAP TO 0
C   HVAP IS IN CALORIES PER GRAM MOLE OF WATER.
C   RECYCLE RATIO IS DEFINED HERE AS THE RATIO OF MOLES OF RECYCLE GAS
C   TO THE MOLES OF FRESH FEED.
C   INITIAL AMOUNTS OF EACH SPECIES FED IN MUST BE GRAM MOLES.

      DIMENSION B(20),Z(20),Y(20),BV(20),BMIN(20),BMAX(20),P(400),A(20,2
     10),AC(20,20)
      DIMENSION BMI(20),BMA(20)
      DIMENSION SLOPE(20),YINTCP(20),HEAT(20)
      DIMENSION SENS2(20),VOL(20),VOLSTP(20)
      DIMENSION ALPHA(20),BETA(20),GAMMA(20),MARK(20),NPR(20)
      DIMENSION DELMOL(20),TGUESSF(40)
      DIMENSION BOX(20),NAME(20),RECY(20)
      DIMENSION FEED(20),RECYL(20),XXN(90,20)
      DIMENSION SPURGE(20),TSPVOL(20),TREVOL(20)
      COMMON/TWO/XN(20),EQUIL(20),STOIC(20,20)
      COMMON/THREE/NS
      COMMON/FOUR/NSOL(20),GAS(20)

      JCOUNT=0
      RECYCLE=0.10
      PRINT 1
      READ 2,NS,NR
      NREACT = NR - 1

      READ 1500,(NAME(J),J=1,NS)
C     NSOL DESIGNATES IF SPECIAL CALCULATIONS REGARDING SOLID-GAS
C     REACTIONS ARE NECESSARY.
C     NSOL=1  MEANS COMPONENT IS A SOLID
C     NSOL=-1  MEANS COMPONENT IS GASEOUS
C     DATA REQUIREMENT---MUST WRITE REACTIONS SO THAT REACTIONS WITH
C     REACTANTS WHICH ARE PRODUCTS OF OTHER REACTIONS APPEAR AFTER ALL
C     THOSE REACTIONS.

C     DATA REQUIREMENT--CONCERNING THIS, THE REACTIONS MUST BE IN
C     IMMEDIATE SEQUENCE.
C     NPR=+1  MEANS THE COMPONENT APPEARS BOTH AS A PRODUCT AND A
C     REACTANT IN THE REACTION SYSTEM BEING STUDIED.
C     NPR=-1  MEANS THE COMPONENT APPEARS ONLY AS REACTANT IN THE
C     REACTION SYSTEM.
      DO 49 I = 1,NS
      READ 3, ALPHA(I), BETA(I), GAMMA(I), MARK(I), NSOL(I), NPR(I)
      PRINT 3003,ALPHA(I),BETA(I),GAMMA(I),MARK(I),NAME(I)
   49 CONTINUE
C  IF MARK IS NEGATIVE CP CONSTANTS FIT THE EQUATION CP = A + BT + C/T**2
```

```
      C  IF MARK IS POSITIVE THE EQUATION CP = A + BT + CT**2 IS USED.
```



```
            PRINT 1501,(NAME(J),J=1,NS)
            DO 50 J = 1,NREACT
            READ 14,(STOIC(J,I),I=1,NS)
            PRINT 4,(STOIC(J,I),I=1,NS)
         50 CONTINUE
      C  THE LAST CARD (ROW) CONTAINS THE INITIAL NUMBER OF GRAM MOLES
      C  FOR EACH SPECIES.
            READ 9,(STOIC(NR,I),I=1,NS)
            PRINT 1502,(NAME(J),J=1,NS)
            PRINT 3007,(STOIC(NR,I),I=1,NS)
            DO 61  J=1,NREACT
            READ 333,SLOPE(J),YINTCP(J),HEAT(J)
        61  CONTINUE
            TSUMT=0.0
            DO 7779 M=1,NS
            FEED(M)=STOIC(NR,M)
            TSUMT=TSUMT+FEED(M)
       7779 CONTINUE

            TREF = 298.0
      C  T1 IS THE FEED TEMPERATURE.
            T1 = TREF
      C  TGUESSF IS THE FLAME TEMPERATURE IN DEGREES FAHRENHEIT.
            JN=1
            TGUESSF(JN)=1940.00
       8999  CONTINUE
       7777 CONTINUE
            JCOUNT=JCOUNT+1
            K1=1
            PRINT 19285, TGUESSF(JN)
      C  TGUESS IS IN DEGREES KELVIN.
            TGUESS=(TGUESSF(JN)-32.0)*5.0/9.0+273.1

            DO 60 J = 1,NREACT
            BMIN(J)=-1000.0
            BMAX(J)=+1000.0
            BV(J) = 1.0
         60 CONTINUE
            PRINT 3005

            IC = 0
            FNU=FLA=TAU=0.0
            EPS=FV=PHMIN=0.0
            NRR=NREACT-1
            ICON=NRR
            KD=NRR
            N=NRR
            KK=NRR
      C  EQUIL(J) ARE THE EQUILIBRIUM CONSTANTS FOR EACH REACTION.
            DO 15 J = 1,NREACT
            EQUIL(J)=10.**(SLOPE(J)/TGUESS + YINTCP(J)  )
            Y(J) = 0.0
```

```
      B(J) = 0.0
   15 CONTINUE
      PRINT 16, (EQUIL(J),J=1,NREACT)
      PRINT 1
```



```
      DO 9911  J=1,NREACT
      DO 9912  JJ=1,NS
      IF (STOIC(J,JJ).LE.1.E-06.AND.STOIC(J,JJ).GE.-1.E-06)  GO TO 9912
      IF (STOIC(J,JJ).LT.-1.E-06.AND.NPR(JJ).GT.0)  GO TO 9600
      IF (STOIC(J,JJ).LT.-1.E-06)  GO TO 9924
      BMI(JJ)=-STOIC(NR,JJ)/STOIC(J,JJ)
      GO TO 1007
 9924 BMA(JJ)=-STOIC(NR,JJ)/STOIC(J,JJ)
      IF(BMAX(J).GE.BMA(JJ))GO TO 1006
      GO TO 1007
 1006 CONTINUE
      BMAX(J)=BMA(JJ)
 1007 IF (STOIC(J,JJ).LT.+1.E-06)  GO TO 1009
      IF(BMIN(J).LE.BMI(JJ))GO TO 1008
      GO TO 1009
 1008 CONTINUE
      BMIN(J)=BMI(JJ)
      GO TO 1009
 9600 BOX(JJ)=0.0
      DO 9601  KA=1,NREACT
      IF (KA.EQ.J)  GO TO 9601
      IF (STOIC(KA,JJ).LT.+1.E-06)  GO TO 9601
      BOX(KA)=-(BMAX(KA)*STOIC(KA,JJ)+STOIC(NR,JJ))/STOIC(J,JJ)
      BOX(JJ)=BOX(JJ)+BOX(KA)
 9601 CONTINUE
      BMA(JJ)=BOX(JJ)
      IF (BMAX(J).GE.BMA(JJ))  BMAX(J)=BMA(JJ)
 1009 CONTINUE
 9912 CONTINUE
 9911 CONTINUE

      DO 801  J=1,NREACT
      PRINT 802, BMIN(J),BMAX(J)
  801 CONTINUE
      B1=BMAX(1)
      BMIN1=BMIN(1)
      EQUIL1=EQUIL(1)
      STO11=STOIC(1,1)
      STO12=STOIC(1,2)
      STO13=STOIC(1,3)
      STOIC(NR,1)=0.0
      STOIC(NR,2)=STOIC(NR,2)-0.5*BMAX(1)
      STOIC(NR,3)=STOIC(NR,3)+BMAX(1)
      DO 5010  J=2,NREACT
      MT=J-1
      EQUIL(MT)=EQUIL(J)
      BMIN(MT)=BMIN(J)
      BMAX(MT)=BMAX(J)
```

```
      DO 5013  I=1,NS
      STOIC(MT,I)=STOIC(J,I)
 5013 CONTINUE
 5010 CONTINUE
C  B(J) ARE THE EXTENTS OF EACH REACTION.
C  Y(J) ARE THE VALUES OF THE NONLINEAR EQUATIONS.
C  BSOLVE IS A SUBROUTINE WHICH SOLVES NN NONLINEAR
```



```
C  EQUATIONS FOR MM UNKNOWNS WHERE MM .LE. NN.
C  DEFINITIONS OF ALL TERMS IN BSOLVE FOUND IN APPENDIX OF
C  MATERIAL AND ENERGY BALANCES BY HENLEY, E.J., AND ROSEN, M.
      I=0
   80 CONTINUE
      CALL BSOLVE (KK,B,N,Z,Y,PH,FNU,FLA,TAU,EPS,PHMIN,I,ICON,FV,DV,BV,B
     1MIN,BMAX,P,FNTX,DERIV,KD,A,AC,GAMM)
      PRINT 3002,FV,ICON,(B(J),J=1,NRR),PH
      IF (FV.GT.300.)  GO TO 75
      IF(ICON)75,75,80
   75 CONTINUE
      PRINT 52,(Z(J),J=1,NRR)
      NREACT=NRR+1
      NR=NREACT+1
      NTR=0
      DO 5011  J=2,NREACT
      MT=NREACT-NTR
      MMT=NREACT-(NTR+1)
      EQUIL(MT)=EQUIL(MMT)
      BMIN(MT)=BMIN(MMT)
      BMAX(MT)=BMAX(MMT)
      B(MT)=B(MMT)
      DO 5014  I=1,NS
      STOIC(MT,I)=STOIC(MMT,I)
 5014 CONTINUE
      NTR=NTR+1
 5011 CONTINUE
      STOIC(1,1)=STO11
      STOIC(1,2)=STO12
      STOIC(1,3)=STO13
      J=1
      DO 5015  I=4,NS
      STOIC(J,I)=0.0
 5015 CONTINUE
      EQUIL(1)=EQUIL1
      B(1)=B1
      BMAX(1)=B1
      BMIN(1)=BMIN1
C     HEAT CAPACITY CALCULATIONS
C   HEAT(J) IS THE HEAT OF REACTION AT 298 KELVIN FOR EACH OF THE
C   REACTIONS USED.  B(J) IS THE EXTENT OF EACH REACTION.
C   SUM4 IS THE TOTAL HEAT OF REACTION, BASED ON STOICHIOMETRIC
C   PROPORTIONS OF REACTANTS.
```

```
C   SUM5 IS THE TOTAL HEAT NECESSARY TO RAISE  THE TEMPERATURE
C   OF THE REACTION PRODUCTS TO THE INCINERATOR TEMPERATURE, TGUESSF.
      HVAP=9700.00
      TGUSF=TGUESSF(JN)
      DO 20 I=1,NS
      IF(MARK(I).LT.0)GOTO10
      SENS2(I)=ALPHA(I)*(TGUESS-TREF)+BETA(I)/2.*(TGUESS**2-TREF**2)+GAM
     1MA(I)/3.*(TGUESS**3 -TREF**3)
      GO TO 30
   10 CONTINUE
      SENS2(I)=ALPHA(I)*(TGUESS-TREF)+BETA(I)/2.*(TGUESS**2-TREF**2)
     1+GAMMA(I)*(1./TGUESS-1./TREF)
   30 CONTINUE
      IF (I.EQ.NS)  SENS2(I)=SENS2(I)+HVAP
   20 CONTINUE
      SUM4=0.
      DO 65 J = 1,NREACT
      SUM4=SUM4+HEAT(J)*B(J)
   65 CONTINUE
      DO 5872 J=1,NREACT
      PRINT 5873, B(J),J
 5872 CONTINUE
      PRINT 5039
      PRINT 5040,(NAME(I),I=1,NS)
      PRINT 5020,(XN(I),I=1,NS)

      SUM5=0.0
      DO 5031  I=1,NS
      SUM5=SUM5+XN(I)*SENS2(I)
 5031 CONTINUE
      SUM4=ABS(SUM4)
      SUM5=ABS(SUM5)
      REC=RECYCLE*TSUMT
      TNSUM=0.0
      DO 5023  J=1,NS
      TNSUM=TNSUM+XN(J)
      RECY(J)=GAS(J)*REC
      RECYL(J)=FEED(J)+RECY(J)
      STOIC(NR,J)=RECYL(J)
 5023 CONTINUE
      PRINT 5041
      PRINT 5020,(RECY(J),J=1,NS)
      IF (TNSUM.GE.REC)  GO TO 5027
      AMAKEUP=REC-TNSUM
      PRINT 5029,AMAKEUP
      GO TO 5028
 5027 PURGE=TNSUM-REC
      PRINT 5030,PURGE
 5028 CONTINUE
      PRINT 19284, SUM4, SUM5
      KXCON=0
      K=JCOUNT
      IF(K.EQ.1) GO TO 7778
      DO 7781 J=1,NS
      XXN(K,J)=RECYL(J)
```

```
      AAA=XXN(K,J)
      BBB=XXN((K-1),J)
      KCOUNT=0
      IF ((ABS(AAA-BBB)).LT.0.1)  KCOUNT=1
      KXCON=KXCON+KCOUNT
      IF (KXCON.EQ.NS)  GO TO 7780
 7781 CONTINUE
 7778 CONTINUE
      IF (K.GT.1)  GO TO 5025
      DO 5024  J=1,NS
      XXN(K,J)=RECYL(J)
```



```
 5024 CONTINUE
 5025 CONTINUE
      PRINT 13, JCOUNT, KXCON
      PRINT 5035
      PRINT 5040,(NAME(I),I=1,NS)
      PRINT 5020,  (STOIC(NR,J),J=1,NS)
      GO TO 7777
 7780 CONTINUE
      PRINT 13, JCOUNT, KXCON
      PRINT 5035
      PRINT 5040,(NAME(I),I=1,NS)
      PRINT 5020, (STOIC(NR,J), J=1,NS)
 8997 SUM5=0.0
      DO 25  I=1,NS
      SUM5=SUM5+XN(I)*SENS2(I)
   25 CONTINUE
      SUM4=ABS(SUM4)
      SUM5=ABS(SUM5)
      K1=K1+1
      IF (K1.GT.2)  GO TO 77
      PRINT 19284, SUM4, SUM5
   77 CONTINUE
C  ADIABATIC TEMPERATURE SEARCH.
      IF (SUM5.GT.(2.*SUM4))  GO TO 9999
      IF (SUM5.GT.(1.5*SUM4))  GO TO 9998
      IF (SUM5.GT.(1.1*SUM4))  GO TO 9997
      IF (SUM5.GT.(1.05*SUM4))  GO TO 9996
      IF (SUM5.LT.(.5*SUM4))  GO TO 9990
      IF (SUM5.LT.(.67*SUM4))  GO TO 9989
      IF (SUM5.LT.(.8*SUM4))  GO TO 9988
      IF (SUM5.LT.(.95*SUM4))  GO TO 9995
      GO TO 9994
 9999 TGUSF=TGUSF-100.
      GO TO 8998
 9998 TGUSF=TGUSF-50.
      GO TO 8998
 9997 TGUSF=TGUSF-25.
      GO TO 8998
 9996 TGUSF=TGUSF-10.
      GO TO 8998
 9990 TGUSF=TGUSF+100.
      GO TO 8998
 9989 TGUSF=TGUSF+50.
      GO TO 8998
 9988 TGUSF=TGUSF+25.
```

```
      GO TO 8998
 9995 TGUSF=TGUSF+10.
      GO TO 8998
 9994 CONTINUE
      JN=JN+1
      TGUESSF(JN)=TGUSF
      TDELT=ABS(TGUESSF(JN)-TGUESSF(JN-1))
      IF (TDELT.GT.25.)  GO TO 8999
      GO TO 8996
 8998 CONTINUE
      TGUS=(TGUSF-32.0) * 5.0/9.0 + 273.1
      DO 71  I=1,NS
      IF (MARK(I).LT.0)  GO TO 73
```



```
      SENS2(I)=ALPHA(I)*(TGUS-TREF)+BETA(I)/2.*(TGUS**2-TREF**2)+GAMMA(I
     1)/3.*(TGUS**3-TREF**3)
      GO TO 72
   73 CONTINUE
      SENS2(I)=ALPHA(I)*(TGUS-TREF)+BETA(I)/2.*(TGUS**2-TREF**2)+GAMMA(I
     1)*(1./TGUS-1./TREF)
   72 CONTINUE
      IF (I.EQ.NS)  SENS2(I)=SENS2(I)+HVAP
   71 CONTINUE
      GO TO 8997
 8996 CONTINUE
C  VOL(I) ARE THE IDEAL GAS VOLUMES OF EACH SPECIES IN CUBIC FEET.
C   XN(I) ARE THE FINAL NUMBER OF GRAM MOLES OF EACH SPECIES AFTER RXN.
      DO 90 I = 1,NS
      VOL(I)=XN(I)*(TGUESSF(JN)+460.0)*(.73/(454.*1.))
      VOLSTP(I)=XN(I)*(77.0+460.0)*(.73/(454.*1.))
   90 CONTINUE
      PRINT 1
      PRINT 12
      PRINT 7, TGUESSF(JN)
      PRINT 19284,SUM4,SUM5
      PRINT 5037
      DO 5038  I=1,NS
      PRINT 5036, NAME(I), FEED(I)
 5038 CONTINUE
      PRINT 1510
      PRINT 5
      PRINT 8
      VOL(1)=0.0
      VOLSTP(1)=0.0
      SU=0.0
      SUU=0.0
      DO 105 I=1,NS
      DELMOL(I)=RECYL(I)-XN(I)
      SPURGE(I)=GAS(I)*PURGE
      TSPVOL(I)=SPURGE(I)*(77.+460.0)*(.73/(454.*1.))
      SU=SU+TSPVOL(I)
      TREVOL(I)=RECY(I)*(77.+460.0)*(.73/(454.*1.))
      SUU=SUU+TREVOL(I)
      PRINT6,NAME(I),STOIC(NR,I),XN(I),DELMOL(I),VOL(I),VOLSTP(I)
```

```
      105 CONTINUE
          PRINT 3005
          PRINT 5045
          PRINT 5040,(NAME(I),I=1,NS)
          PRINT 5020,(SPURGE(I),I=1,NS)
          PRINT 5020,(TSPVOL(I),I=1,NS)
          PRINT 5020,(TREVOL(I),I=1,NS)
          PRINT 5046,SU
          PRINT 5047,SUU

          CALL EXIT

        1 FORMAT(1H1)
```



```
        2 FORMAT(2I3)
      3   FORMAT(3E10.3,3I2)
       4  FORMAT (15(2X,F4.1)/)
        5 FORMAT(//, 7X,*SPECIES*,5X,*INITIAL*,10X,*FINAL*,10X,*CHANGE*,10X,*GAS,10X
         1*GAS*,10X,*IDEAL*)
      6   FORMAT(10X,A4,5(5X,E10.3)/)
        7 FORMAT(////*                FLAME TEMPERATURE = *,F8.1,* DEGREES FAHRENH
         1EIT*///)
        8 FORMAT( 7X,*SYMBOL*,6X,*MOLES*,12X,*MOLES*,10X,*MOLES*,11X,*VOLUME
         1*,7X,*VOLUME*//)
      9   FORMAT(14F5.2)
      12  FORMAT (///*                FINAL DATA SUMMARY*)
       13 FORMAT(25X,* COMPOSITION AFTER CYCLE*,2X,I3,/,25X,
         1 * NUMBER OF SATISFIED COMPONENTS*,2X,I4,//)
      14  FORMAT(20F4.1)
      16  FORMAT( 25X,*EQUILIBRIUM CONSTANTS*,/10(2X,E10.3))
      52  FORMAT (7E14.2)
      333 FORMAT (3E10.3)
      802 FORMAT(*  BMIN(J)=  *,F15.8,*  BMAX(J)=  *,F15.8)
     1500 FORMAT(20A4)
     1501 FORMAT(15(2X,A4)//)
     1502 FORMAT (/,14(4X,A4))
     1510 FORMAT( 25X,*FINAL EQUILIBRIUM COMPOSITIONS*)
     3002 FORMAT (1X,F5.0,I5,14(E8.1))
     3003 FORMAT(3(10X,E10.3),10X,I3,10X,A4,/)
     3005 FORMAT(  ///)
     3007 FORMAT (/,14(1X,F7.3))
     5020 FORMAT (13E9.2,/)
     5029 FORMAT(*  EXTRA OFF GAS REQUIRED FOR RECYCLE = *,E10.2)
     5030 FORMAT(*  MOLES TO BE PURGED = *,E10.2)
     5035 FORMAT (10X,*  THE TOTAL FEED IS  *)
     5036 FORMAT (10X,A4,5X,E10.2,*  MOLES*)
     5037 FORMAT (10X,*  THE FRESH FEED IS*)
     5039 FORMAT (/,*  PRODUCTS OF THE REACTIONS ARE AS FOLLOWS*)
     5040 FORMAT (/,13(5X,A4))
     5041 FORMAT (/,*    AMOUNTS OF EACH SPECIES TO BE RECYCLED*)
     5045 FORMAT (*  BELOW ARE LISTED RESPECTIVELY, FOR EACH SPECIES, GRAM
         1MOLES PURGED, AND STP VOLUME OF AMOUNTS PURGED AND RECYCLED.*)
     5046 FORMAT (//,*  THE TOTAL STP VOLUME TO BE PURGED IS *,E11.3)
     5047 FORMAT (//,*  THE TOTAL STP VOLUME TO BE RECYCLED IS *,E11.3)
     5873 FORMAT (/.10X,F14.6,*  = EXTENT OF REACTION *,I3)
```

```
19284 FORMAT(10X,*HEAT OF REACTION= *,E10.3,/,10X,*HEAT FOR TEMP RISE= *
     1,E10.3)
19285 FORMAT(10X,*TGUESSF= *,F10.2)
      END
          TRACE                              CDC 6600 FTN V3.0-P336 OPT=0  07/10/73  12.25.48.       PAGE    1
*DECK BSOLVE
      SUBROUTINE BSOLVE(KK,B,NN,Z,Y,PH,FNU,FLA,TAU,EPS,
     1                PHMIN,I,ICON,FV,DV,BV,BMIN,BMAX,P,
     2                FUNC,DERIV,KD,A,AC,GAMM)


C     SOLUTION OF NN EQUATIONS IN KK UNKNOWNS BY MARQUARDTS METHOD.
      DIMENSION B(20),Z(20),Y(20),FV(20),DV(20),BV(20),BMIN(20),
     1          BMAX(20),P(400),A(KD,4),AC(KD,4)
      K = KK
      N = NN
      KP1 = K + 1
      KP2 = KP1 + 1
      KBI1 = K * N
      KBI2 = KBI1 + K
      KZI = KBI2 + K
      IF( FNU .LE. 0.0 )FNU = 10.0
      IF( FLA .LE. 0.0 ) FLA = 0.01
      IF( TAU .LE. 0.0 ) TAU = 0.001
      IF( EPS .LE. 0.0 ) EPS = 0.00002
      IF( PHMIN .LE. 0.0 ) PHMIN = 0.0
  120 KE = 0
  130 DO 160 I1 = 1,K
  160 IF( BV(I1) .NE. 0.0 ) KE = KE + 1
      IF( KE .GT. 0 ) GO TO 170
  162 ICON=-3
  163 GO TO 2120
  170 IF(N.GE.KE) GO TO 500
  180 ICON=-2
  190 GO TO 2120
  500 I1 = 1
  530 IF( I .GT. 0 ) GO TO 1530
  550 DO 560 J1 = 1 , K
      J2 = KBI1 + J1
      P(J2) = B(J1)
      J3 = KBI2 + J1

560   P(J3)=ABS(B(J1))+1.0E-02
      GO TO 1030
  590 IF( PHMIN .GT. PH .AND.  I .GT. 1 ) GO TO 625
      DO 620 J1 = 1 , K
      N1 = (J1 - 1) * N
      IF( BV(J1) ) 601,620,605
  601 CALL DERIV  (K,B,N,Z,P(N1+1),FV,DV,J1,JTEST)
      IF( JTEST .NE. (-1) ) GO TO 620
      BV(J1) = 1.0
  605 DO 606 J2 = 1,K
      J3 = KBI1 + J2
  606 P(J3) = B(J2)
      J3 = KBI1 + J1
```

```
      J4 = KBI2 + J1
      SORE=ABS(P(J3))
      QQQ = AMAX1(P(J4),SORE)
      DEN=.001*QQQ
      IF(P(J3) + DEN .LE. BMAX(J1) ) GO TO 55
         P(J3) = P(J3) - DEN
         DEN = - DEN
```


```
      GO TO 56
55    P(J3)= P(J3) + DEN
   56 CALL FUNC  (K,P(KBI1+1),N,P(N1+1),FV)
      DO 610 J2=1,N
      JB = J2 + N1
  610 P(JB) = ( P(JB) - Z(J2) ) / DEN
  620 CONTINUE
C
C        SET UP CORRECTION EQUATIONS

  625 DO 725 J1 = 1 , K
      N1 = (J1-1) * N
      A(J1,KP1) = 0.
      IF( BV(J1) ) 630,692,630
  630 DO 640 J2 = 1,N
      N2 = N1 + J2
  640 A(J1,KP1) = A(J1,KP1) + P(N2) * ( Y(J2) - Z(J2) )
  650 DO 680 J2 = 1 , K
  660 A(J1,J2) = 0.
  665 N2 = (J2-1) * N
  670 DO 680 J3 = 1 , N
  672 N3 = N1 + J3
  674 N4 = N2 + J3
  680 A(J1,J2) = A(J1,J2) + P(N3) * P(N4)
      IF( A(J1,J1) .GT. 1.E-20 )GO TO 725
  692 DO 694 J2 = 1,KP1
  694 A(J1,J2) = 0.
  695 A(J1,J1) = 1.0
  725 CONTINUE
      GN = 0.
      DO 729 J1 = 1,K
  729 GN = GN + A(J1,KP1)**2
C         SCALE CORRECTION EQUATIONS

      DO 726 J1 = 1,K
  726 A(J1,KP2) = SQRT(A(J1,J1))
      DO 727 J1 = 1,K
      A(J1,KP1) = A(J1,KP1) / A(J1,KP2)
      DO 727 J2 = 1,K
  727 A(J1,J2) = A(J1,J2) / (A(J1,KP2) * A(J2,KP2) )
  730 FL = FLA / FNU
      GO TO 810
800   FL=FNU*FL
  810 DO 840 J1 = 1,K
  820 DO 830 J2 = 1,KP1
  830 AC(J1,J2) = A(J1,J2)
  840 AC(J1,J1) = AC(J1,J1) + FL
C         SOLVE CORRECTION EQUATIONS
```

```
      DO 930 L1 = 1,K
      L2 = L1 + 1
      DO 910 L3 = L2,KP1
  910 AC(L1,L3) = AC(L1,L3) / AC(L1,L1)
      DO 930 L3 = 1,K
      IF(L1 - L3) 920,930,920
  920 DO 925 L4 = L2,KP1
  925 AC(L3,L4) = AC(L3,L4) - AC(L1,L4) * AC(L3,L1)
```



```
  930 CONTINUE

      DN = 0.
      DG = 0.
      DO 1028 J1 = 1,K
      AC(J1,KP2) = AC(J1,KP1) / A(J1,KP2)
      J2 = KBI1 + J1
      P(J2) = AMAX1(BMIN(J1),AMIN1(BMAX(J1),B(J1)+AC(J1,KP2)))
         DG = DG + AC(J1,KP2) * A(J1,KP1) * A(J1,KP2)
      DN = DN + AC(J1,KP2) * AC(J1,KP2)
 1028 AC(J1,KP2) = P(J2) - B(J1)
      COSG = DG / SQRT(DN*GN)
      JGAM = 0
      IF( COSG ) 1100,1110,1110
 1100 JGAM = 2
      COSG = -COSG
 1110 CONTINUE
         COSG = AMIN1(COSG,1.0)
      GAMM = ARCOS(COSG) * 180. / (3.14159265)
      IF( JGAM .GT. 0 ) GAMM = 180. - GAMM
 1030 CALL FUNC  (K,P(KBI1+1),N,P(KZI+1),FV)
 1500 PHI = 0.
      DO 1520 J1 = 1,N
      J2 = KZI + J1
 1520 PHI = PHI + (F(J2) - Y(J1))**2
      IF(PHI .LT. 1.E-10 ) GO TO 3000
      IF( I .GT. 0 ) GO TO 1540
 1521 ICON = K
      GO TO 2110
 1540 IF( PHI .GE. PH ) GO TO 1530

C     EPSILON TEST

 1200 ICON = 0
      DO 1220 J1 = 1,K
      J2 = KBI1 + J1
      CRA=ABS(AC(J1,KP2))
      CRB=ABS(P(J2))+TAU
      CRC=CRA/CRB
 1220 IF (CRC.GT.EPS)  ICON=ICON+1
      IF( ICON .EQ. 0 ) GO TO 1400

C        GAMMA LAMBDA TEST

      IF( FL .GT. 1.0 .AND. GAMM .GT. 90.0 ) ICON = -1
      GO TO 2105
```

```
      C         GAMMA EPSILON TEST
        1400 IF(FL .GT. 1.0 .AND. GAMM .LE. 45.0) ICON = -4
             GO TO 2105

        1530 IF( I1 - 2 ) 1531,1531,2310
        1531 I1 = I1+ 1
             GO TO (530,590,800),I1
        2310 IF( FL .LT. 1.0E+08 ) GO TO 800
        1320 ICON = -1
 SUBROUTINE  BSOLVE    TRACE                 CDC 6600 FTN V3.0-P336 OPT=0  07/10/73  12.25.48.      PAGE     4
        2105 FLA = FL
             DO 2091 J2 = 1,K
             J3 = KBI1 + J2
        2091 B(J2) = P(J3)
        2110 DO 2050 J2 = 1,N
             J3 = KZI + J2
        2050 Z(J2) = P(J3)
             PH = PHI
             I = I + 1
        2120 RETURN
        3000 ICON = 0
             GO TO 2105
             END
                   TRACE                     CDC 6600 FTN V3.0-P336 OPT=0  07/10/73  12.25.48.      PAGE     1

      *DECK FNTX
              SUBROUTINE  FNTX (KK,B,NN,Z,FV)
             DIMENSION B(20),Z(20),SUM(20)
             COMMON/TWO/XN(20),EQUIL(20),STOIC(20,20)
             COMMON/THREE/NS
             COMMON/FOUR/NSOL(20),GAS(20)
             NREACT = KK
             NR=NREACT+2
             FV = FV + 1.0
             SUMG=0.0
      C      SOLIDS CRUTCH
             DO 30 I = 1,NS
             XN(I) = STOIC(NR,I)
             DO 40 J = 1,NREACT
             XN(I) = XN(I) + STOIC(J,I) * B(J)
          40 CONTINUE
             IF (NSOL(I).GT.0)  GO TO 30
             SUMG = SUMG + XN(I)
          30 CONTINUE

             DO 85  I=1,NS
             GAS(I) = XN(I) / SUMG
             IF (GAS(I).LT.1.E-09)  GAS(I)=1.E-09
          85 CONTINUE
             DO 60 J = 1,NREACT
             SUM(J) = 0.0
             DO 70  I=1,NS
             SUM(J) = SUM(J) + STOIC(J,I) * ALOG(GAS(I))
```

```
      70 CONTINUE
      60 CONTINUE
         DO 80 J = 1,NREACT
C        END SOLIDS CRUTCH
         Z(J) = -ALOG(EQUIL(J)) + SUM(J)
      80 CONTINUE
         RETURN
         END
              TRACE                      CDC 6600 FTN V3.0-P336 OPT=0  07/10/73  12.25.48.       PAGE     1
*DECK ARCOS
         FUNCTION ARCOS(Z)
         X = Z
         KEY = 0
         IF( X .LT. (-1.) ) X = -1.
         IF( X .GT. 1. ) X = 1.
         IF( X .GE. (-1.) .AND. X .LT. 0. ) KEY = 1
         IF( X .LT. 0.) X = ABS(X)
         IF( X .EQ. 0. ) GO TO 10
         ARCOS = ATAN (SQRT(1. - X*X) / X )
         IF( KEY .EQ. 1) ARCOS = 3.14159265 - ARCOS
         GO TO 999
      10 ARCOS = 1.5707963
     999 RETURN
         END
 FUNCTION    AMIN1    TRACE              CDC 6600 FTN V3.0-P336 OPT=0  07/10/73  12.25.48.       PAGE     1
         FUNCTION AMIN1(A,B)
         AMIN1=B
         IF (A.LT.B)  AMIN1=A
         RETURN
         END
              TRACE                      CDC 6600 FTN V3.0-P336 OPT=0  07/10/73  12.25.49.       PAGE     1
         FUNCTION AMAX1(A,B)
         AMAX1=B
         IF (A.GT.B)  AMAX1=A
         RETURN
         END
CORE MAP  12.26.18.  NORMAL            CONTROL                                000100     027550     000000     000000
      ---TIME---LOAD MODE --L1--L2-----TYPE---------------USER---++---CALL-------------FWA LOAD--LWA LOAD--BLNK COMN--LENGTH--
      FWA LOADER  062733  FWA TABLES  062422
      -PROGRAM----ADDRESS-                  --LABELED---COMMON----ADDRESS-
      GARBAGE     001041                              TWO         000100
                                                      THREE       000770
                                                      FOUR        000771
      BSOLVE      016757
      FNTX        020503                              TWO         000100
                                                      THREE       000770
                                                      FOUR        000771
      ARCOS       020721
      AMIN1       021020
      AMAX1       021037
      GETBA       021056
      STO$        021075
      SYSTEM$     022546
      ACGOER$     023557
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INPUTC$     023572
KODER$      023726
KRAKER$     025345
OUTPTC$     027072
ABS$        027166
ALNLOGE     027171
ALOG$       027230
ATAN$       027262
ATANE       027302
EXPE        027363
SQRT$       027427
SQRTE       027453
XTOY$       027475
----UNSATISFIED EXTERNALS-----                                REFERENCES

     .403E+01        .114E-02        -.204E+06        -1        C(S)
     .615E+01        .310E-02        -.923E-06         1        O2
     .642E+01        .166E-02        -.196E-06         1        CO
     .621E+01        .104E-01        -.354E-05         1        CO2
     .683E+01        .900E-03        -.120E+05        -1        N2
     .703E+01        .920E-03        -.140E+05        -1        NO
     .101E+02        .228E-02        -.167E+06        -1        NO2
     .652E+01        .780E-03         .120E+05        -1        H2
     .526E+01       -.100E-03         .360E+05        -1        S
     .110E+02        .188E-02        -.184E+06        -1        SO2
     .139E+02        .610E-02        -.322E+06        -1        SO3
     .666E+01        .513E-02        -.854E-06         1        H2S
     .730E+01        .246E-02        0.               -1        H2O
C(S)   O2    CO    CO2   N2    NO    NO2   H2    S     SO2   SO3   H2S   H2O
-1.0   -.5   1.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0
-0.0   -.5  -1.0   1.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0
-0.0   -.5  -0.0  -0.0   -.5   1.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0
-0.0   -.5  -0.0  -0.0  -0.0  -1.0   1.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0
-0.0   -.5  -0.0  -0.0  -0.0  -0.0  -0.0  -1.0  -0.0  -0.0  -0.0  -0.0   1.0
-0.0  -1.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -1.0   1.0  -0.0  -0.0  -0.0
-0.0   -.5  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -1.0   1.0  -0.0  -0.0
-0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -1.0  -1.0  -0.0  -0.0   1.0  -0.0
   C(S)     O2       CO       CO2      N2       NO       NO2      H2       S        SO2      SO3      H2S      H2O

  8.140   11.730   -0.000   -0.000   38.160   -0.000   -0.000   5.940    .020   -0.000   -0.000   -0.000   15.160
        TGUESSF=     1940.00
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                                   EQUILIBRIUM CONSTANTS
    .122E+10      .267E+07      .135E-02      .436E-01      .711E+07      .843E+01      .283E-02      .768E+07

   BMIN(J)=        -0.00000000   BMAX(J)=         8.14000000
   BMIN(J)=        -0.00000000   BMAX(J)=         8.14000000
   BMIN(J)=        -0.00000000   BMAX(J)=        23.40000000
   BMIN(J)=        -0.00000000   BMAX(J)=        23.40000000
   BMIN(J)=       -15.16000000   BMAX(J)=         5.94000000
   BMIN(J)=        -0.00000000   BMAX(J)=          .02000000
   BMIN(J)=        -0.00000000   BMAX(J)=          .02000000
   BMIN(J)=        -0.00000000   BMAX(J)=          .02000000
     1.     7 0.        0.        0.        0.        0.        0.        0.        .2E+04
     9.     7  .6E-04   .2E-04   .1E-04   .6E+01   .2E-04   .2E-05   .4E-04   .8E+03
    17.     7  .2E-02   .3E-03   .6E-04   .6E+01   .2E-03   .9E-05   .3E-03   .7E+03
    25.     7  .4E-01   .1E-02   .1E-03   .6E+01   .9E-03   .5E-05   .2E-02   .4E+03
    33.     7  .8E+00   .5E-02   .2E-03   .6E+01   .3E-02   .4E-05   .5E-02   .3E+03
    41.     7  .8E+01   .8E-02-0.          .6E+01   .6E-03-0.          .1E-01   .1E+03
    59.     5  .9E+01   .7E-02   .1E-06   .6E+01   .6E-03   .2E-07   .1E-01   .1E+03
    67.     6  .8E+01   .6E-02   .1E-05   .6E+01   .5E-03   .2E-06   .1E-01   .7E+02
    75.     7  .8E+01   .3E-02   .7E-05   .6E+01   .4E-03-0.          .2E-01   .2E+02
    86.     4  .8E+01   .3E-02   .7E-05   .6E+01   .4E-03   .9E-08   .2E-01   .2E+02
    95.     4  .8E+01   .3E-02   .7E-05   .6E+01   .4E-03   .2E-07   .2E-01   .2E+02
   104.     4  .8E+01   .3E-02   .7E-05   .6E+01   .4E-03   .3E-07   .2E-01   .2E+02
   113.     4  .8E+01   .3E-02   .7E-05   .6E+01   .4E-03   .4E-07   .2E-01   .1E+02
   122.     4  .8E+01   .3E-02   .7E-05   .6E+01   .4E-03   .5E-07   .2E-01   .1E+02
   131.     4  .8E+01   .3E-02   .7E-05   .6E+01   .4E-03   .5E-07   .2E-01   .1E+02
   140.     4  .8E+01   .3E-02   .8E-05   .6E+01   .4E-03   .6E-07   .2E-01   .1E+02
   149.     4  .8E+01   .3E-02   .8E-05   .6E+01   .4E-03   .7E-07   .2E-01   .1E+02
   158.     3  .8E+01   .3E-02   .8E-05   .6E+01   .4E-03   .8E-07   .2E-01   .9E+01
   167.     4  .8E+01   .3E-02   .8E-05   .6E+01   .4E-03   .8E-07   .2E-01   .8E+01
   176.     4  .9E+01   .3E-02   .8E-05   .6E+01   .4E-03   .9E-07   .2E-01   .7E+01
   185.     4  .8E+01   .3E-02   .8E-05   .6E+01   .4E-03   .9E-07   .2E-01   .6E+01
   194.     4  .8E+01   .3E-02   .8E-05   .6E+01   .4E-03   .9E-07   .2E-01   .5E+01
   203.     4  .8E+01   .3E-02   .8E-05   .6E+01   .4E-03   .1E-06   .2E-01   .4E+01
   212.     3  .8E+01   .3E-02   .8E-05   .6E+01   .4E-03   .1E-06   .2E-01   .4E+01
   221.     3  .8E+01   .3E-02   .8E-05   .6E+01   .4E-03   .1E-05   .2E-01   .3E+01
   230.     3  .8E+01   .3E-02   .8E-05   .6E+01   .4E-03   .1E-06   .2E-01   .3E+01
   239.     3  .8E+01   .3E-02   .8E-05   .6E+01   .4E-03   .1E-06   .2E-01   .3E+01
   248.     3  .8E+01   .3E-02   .8E-05   .6E+01   .4E-03   .1E-06   .2E-01   .3E+01
   257.     3  .8E+01   .3E-02   .8E-05   .6E+01   .4E-03   .1E-06   .2E-01   .3E+01
   265.     4  .8E+01   .4E-02   .9E-05   .6E+01   .3E-03   .9E-07   .2E-01   .2E+01
   275.     3  .8E+01   .4E-02   .9E-05   .6E+01   .3E-03   .9E-07   .2E-01   .2E+01
   283.     3  .8E+01   .4E-02   .1E-04   .6E+01   .3E-03   .9E-07   .2E-01   .2E+01
   293.     3  .8E+01   .4E-02   .1E-04   .6E+01   .3E-03   .9E-07   .2E-01   .2E+01
   302.     3  .8E+01   .4E-02   .1E-04   .6E+01   .3E-03   .9E-07   .2E-01   .2E+01
      -.18E+00        -.60E+00        -.39E+00        -.55E+00        .93E+00        .57E-02        .52E+00

                  8.140000  = EXTENT OF REACTION   1

                  8.139961  = EXTENT OF REACTION   2

                   .003562  = EXTENT OF REACTION   3

                   .000010  = EXTENT OF REACTION   4

                  5.921995  = EXTENT OF REACTION   5
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.000324 = EXTENT OF REACTION 6

.000000 = EXTENT OF REACTION 7

.017950 = EXTENT OF REACTION 8

PRODUCTS OF THE REACTIONS ARE AS FOLLOWS

C(S)	O2	CO	CO2	N2	NO	NO2	H2	S	SO2	SO3	H2S	H2O
0.	.60E+00	.39E-04	.81E+01	.38E+02	.36E-02	.98E-05	.55E-04	.17E-02	.32E-03	.86E-07	.18E-01	.21E+02

AMOUNTS OF EACH SPECIES TO BE RECYCLED

.79E-08	.69E-01	.45E-05	.95E+00	.44E+01	.41E-03	.11E-05	.64E-05	.20E-03	.38E-04	.10E-07	.21E-02	.25E+01

MOLES TO BE PURGED = .60E+02
HEAT OF REACTION= .111E+07
HEAT FOR TEMP RISE= .814E+06
COMPOSITION AFTER CYCLE 1
NUMBER OF SATISFIED COMPONENTS 0

THE TOTAL FEED IS

C(S)	O2	CO	CO2	N2	NO	NO2	H2	S	SO2	SO3	H2S	H2O
.81E+01	.12E+02	.45E-05	.95E+00	.43E+02	.41E-03	.11E-05	.59E+01	.20E-01	.38E-04	.10E-07	.21E-02	.18E+02

TGUESSF= 1940.00

EQUILIBRIUM CONSTANTS

.122E+10	.267E+07	.135E-02	.436E-01	.711E+07	.843E+01	.283E-02	.768E+07

BMIN(J)=	-.00000452	BMAX(J)=	8.14000001
BMIN(J)=	-.94709809	BMAX(J)=	8.14000452
BMIN(J)=	-.00341332	BMAX(J)=	23.53890333
BMIN(J)=	-.00000114	BMAX(J)=	23.53890333
BMIN(J)=	-17.61292531	BMAX(J)=	5.94000639
BMIN(J)=	-.00003774	BMAX(J)=	.02020072
BMIN(J)=	-.00000001	BMAX(J)=	.02023847
BMIN(J)=	-.00208856	BMAX(J)=	.02020072

1.	7	0.	0.	0.	0.	0.	0.	0.	.7E+03
9.	6	.8E+01	.9E-03	.8E-05	.6E+01	.7E-04	-.1E-07	.1E-01	.1E+03
23.	5	.8E+01	.9E-03	.7E-05	.6E+01	.7E-04	-.1E-07	.1E-01	.8E+02
31.	5	.8E+01	.1E-02	.7E-05	.6E+01	.8E-04	-.1E-07	.2E-01	.6E+02
40.	5	.8E+01	.1E-02	.7E-05	.6E+01	.9E-04	-.1E-07	.2E-01	.5E+02
50.	4	.8E+01	.1E-02	.7E-05	.6E+01	.9E-04	-.1E-07	.2E-01	.5E+02
59.	4	.8E+01	.1E-02	.7E-05	.6E+01	.9E-04	-.1E-07	.2E-01	.5E+02
68.	4	.8E+01	.1E-02	.7E-05	.6E+01	.9E-04	-.1E-07	.2E-01	.4E+02
77.	4	.8E+01	.1E-02	.7E-05	.6E+01	.9E-04	-.1E-07	.2E-01	.4E+02
85.	5	.8E+01	.1E-02	.6E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.4E+02
93.	6	.8E+01	.2E-02	.8E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.2E+02
104.	3	.8E+01	.2E-02	.8E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.2E+02
113.	3	.8E+01	.2E-02	.8E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.2E+02
122.	3	.8E+01	.2E-02	.8E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.2E+02

131.	3	.8E+01	.2E-02	.8E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.2E+02
140.	3	.8E+01	.2E-02	.8E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.2E+02
149.	2	.8E+01	.2E-02	.8E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.2E+02
158.	2	.8E+01	.2E-02	.8E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.2E+02
167.	2	.8E+01	.2E-02	.8E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.1E+02
176.	2	.8E+01	.2E-02	.8E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.1E+02
185.	2	.8E+01	.2E-02	.8E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.1E+02
194.	2	.8E+01	.2E-02	.9E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.1E+02
203.	2	.8E+01	.2E-02	.9E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.1E+02
212.	3	.8E+01	.2E-02	.9E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.9E+01
221.	3	.8E+01	.2E-02	.9E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.9E+01
230.	3	.8E+01	.2E-02	.9E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.8E+01
239.	3	.8E+01	.2E-02	.9E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.7E+01
248.	3	.8E+01	.2E-02	.9E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.7E+01
257.	3	.8E+01	.2E-02	.9E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.7E+01
266.	3	.8E+01	.2E-02	.9E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.6E+01
275.	3	.8E+01	.2E-02	.9E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.6E+01
283.	4	.8E+01	.2E-02	.9E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.5E+01
292.	4	.8E+01	.2E-02	.9E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.5E+01
302.	3	.8E+01	.2E-02	.9E-05	.6E+01	.1E-03	-.1E-07	.2E-01	.5E+01

-.93E+00 -.91E+00 -.15E+00 -.12E+01 .70E+00 .70E+00 .60E+00

8.140000 = EXTENT OF REACTION 1

8.139913 = EXTENT OF REACTION 2

.002494 = EXTENT OF REACTION 3

.000009 = EXTENT OF REACTION 4

5.920735 = EXTENT OF REACTION 5

.004104 = EXTENT OF REACTION 6

-.000000 = EXTENT OF REACTION 7

.019150 = EXTENT OF REACTION 8

PRODUCTS OF THE REACTIONS ARE AS FOLLOWS

C(S)	O2	CO	CO2	N2	NO	NO2	H2	S	SO2	SO3	H2S	H2O
0.	.67E+00	.92E-04	.91E+01	.43E+02	.29E-02	.10E-04	.12E-03	.95E-03	.14E-03	0.	.21E-01	.24E+02

AMOUNTS OF EACH SPECIES TO BE RECYCLED

.79E-08	.70E-01	.96E-05	.95E+00	.44E+01	.30E-03	.11E-05	.13E-04	.99E-04	.15E-04	.79E-08	.22E-02	.25E+01

MOLES TO BE PURGED = .68E+02
HEAT OF REACTION= .111E+07
HEAT FOR TEMP RISE= .939E+06
COMPOSITION AFTER CYCLE 2
NUMBER OF SATISFIED COMPONENTS 13

THE TOTAL FEED IS

C(S)	O2	CO	CO2	N2	NO	NO2	H2	S	SO2	SO3	H2S	H2O
.81E+01	.12E+02	.96E-05	.95E+00	.43E+02	.30E-03	.11E-05	.59E+01	.20E-01	.15E-04	.79E-08	.22E-02	.18E+02

HEAT OF REACTION= .111E+07
HEAT FOR TEMP RISE= .909E+06
TGUESSF= 2300.00

EQUILIBRIUM CONSTANTS

.317E+09 .974E+05 .390E-02 .203E-01 .380E+06 .156E+01 .198E-03 .445E+07

BMIN(J)=	-.00000957	BMAX(J)=	8.14000301
BMIN(J)=	-.94709708	BMAX(J)=	8.14000957
BMIN(J)=	-.00030211	BMAX(J)=	23.53919762
BMIN(J)=	-.00000106	BMAX(J)=	23.53919762
BMIN(J)=	-17.61280446	BMAX(J)=	5.94001273
BMIN(J)=	-.00001477	BMAX(J)=	.02009872
BMIN(J)=	-.00000001	BMAX(J)=	.02011349
BMIN(J)=	-.00221355	BMAX(J)=	.02009872

1.	7	0.	0.	0.	0.	0.	0.	0.	.6E+03
9.	6	.8E+01	.1E-02	.1E-04	.6E+01	.1E-04	-.8E-08	.2E-01	.3E+03
21.	6	.8E+01	.3E-02	.2E-04	.4E+01	.6E-04	-.8E-08	.1E-01	.2E+03
31.	6	.8E+01	.3E-02	.1E-04	.5E+01	.7E-04	-.8E-08	.2E-01	.2E+03
40.	6	.8E+01	.4E-02	.1E-04	.6E+01	.9E-04	-.8E-08	.2E-01	.1E+03
49.	6	.8E+01	.4E-02	.1E-04	.6E+01	.1E-03	-.8E-08	.2E-01	.1E+03
58.	6	.8E+01	.4E-02	.1E-04	.6E+01	.1E-03	-.8E-08	.2E-01	.8E+02
67.	5	.8E+01	.5E-02	.1E-04	.6E+01	.1E-03	-.8E-08	.2E-01	.6E+02
76.	5	.8E+01	.5E-02	.1E-04	.6E+01	.1E-03	-.8E-08	.2E-01	.5E+02
85.	5	.8E+01	.6E-02	.1E-04	.6E+01	.1E-03	-.8E-08	.2E-01	.5E+02
94.	5	.8E+01	.6E-02	.1E-04	.6E+01	.1E-03	-.8E-08	.2E-01	.4E+02
103.	5	.8E+01	.6E-02	.1E-04	.6E+01	.1E-03	-.8E-08	.2E-01	.4E+02
112.	5	.8E+01	.7E-02	.1E-04	.6E+01	.1E-03	-.8E-08	.2E-01	.3E+02
120.	5	.8E+01	.9E-02	.1E-04	.6E+01	.1E-03	-.8E-08	.2E-01	.2E+02
129.	5	.8E+01	.1E-01	.2E-04	.6E+01	.9E-04	-.8E-08	.2E-01	.2E+02
138.	5	.8E+01	.1E-01	.2E-04	.6E+01	.8E-04	-.8E-08	.2E-01	.2E+02
147.	5	.8E+01	.1E-01	.2E-04	.6E+01	.8E-04	-.8E-08	.2E-01	.2E+02
156.	5	.8E+01	.2E-01	.3E-04	.6E+01	.8E-04	-.8E-08	.2E-01	.2E+02
165.	4	.8E+01	.2E-01	.3E-04	.6E+01	.8E-04	-.8E-08	.2E-01	.2E+02
174.	4	.8E+01	.2E-01	.3E-04	.6E+01	.8E-04	-.8E-08	.2E-01	.2E+02
183.	4	.8E+01	.2E-01	.3E-04	.6E+01	.8E-04	-.8E-08	.2E-01	.2E+02
192.	4	.8E+01	.2E-01	.3E-04	.6E+01	.8E-04	-.8E-08	.2E-01	.2E+02
201.	4	.8E+01	.2E-01	.3E-04	.6E+01	.9E-04	-.8E-08	.2E-01	.2E+02
210.	4	.8E+01	.2E-01	.3E-04	.6E+01	.9E-04	-.8E-08	.2E-01	.2E+02
219.	4	.8E+01	.2E-01	.3E-04	.6E+01	.9E-04	-.8E-08	.2E-01	.2E+02
228.	4	.8E+01	.2E-01	.4E-04	.6E+01	.9E-04	-.8E-08	.2E-01	.2E+02
237.	4	.8E+01	.2E-01	.4E-04	.6E+01	.9E-04	-.8E-08	.2E-01	.2E+02
246.	4	.8E+01	.2E-01	.4E-04	.6E+01	.9E-04	-.8E-08	.2E-01	.2E+02
255.	4	.8E+01	.2E-01	.4E-04	.6E+01	.1E-03	-.8E-08	.2E-01	.2E+02
264.	4	.8E+01	.2E-01	.4E-04	.6E+01	.1E-03	-.8E-08	.2E-01	.2E+02
273.	4	.8E+01	.2E-01	.4E-04	.6E+01	.1E-03	-.8E-08	.2E-01	.2E+02
282.	4	.8E+01	.2E-01	.4E-04	.6E+01	.1E-03	-.8E-08	.2E-01	.2E+02
291.	4	.8E+01	.2E-01	.4E-04	.6E+01	.1E-03	-.8E-08	.2E-01	.2E+02
300.	4	.8E+01	.2E-01	.4E-04	.6E+01	.1E-03	-.8E-08	.2E-01	.2E+02
309.	4	.8E+01	.2E-01	.4E-04	.6E+01	.1E-03	-.8E-08	.2E-01	.2E+02

-.81E-02 -.45E-01 -.83E-03 .57E+00 .17E+01 .36E+01 -.58E+00

6.140900 = EXTENT OF REACTION 1

8.139000 = EXTENT OF REACTION 2

.019495 = EXTENT OF REACTION 3

.000036 = EXTENT OF REACTION 4

5.921304 = EXTENT OF REACTION 5

.000103 = EXTENT OF REACTION 6

-.000000 = EXTENT OF REACTION 7

.018332 = EXTENT OF REACTION 8

PRODUCTS OF THE REACTIONS ARE AS FOLLOWS

C(S)	O2	CO	CO2	N2	NO	NO2	H2	S	SO2	SO3	H2S	H2O
0.	.66E+00	.10E-02	.91E+01	.43E+02	.20E-01	.37E-04	.38E-03	.17E-02	.12E-03	0.	.21E-01	.24E+02

AMOUNTS OF EACH SPECIES TO BE RECYCLED

.79E-08	.69E-01	.11E-03	.95E+00	.44E+01	.21E-02	.39E-05	.39E-04	.17E-03	.12E-04	.79E-08	.21E-02	.25E+01

MOLES TO BE PURGED = .68E+02
HEAT OF REACTION= .111E+07
HEAT FOR TEMP RISE= .106E+07
COMPOSITION AFTER CYCLE 3
NUMBER OF SATISFIED COMPONENTS 13

THE TOTAL FEED IS

C(S)	O2	CO	CO2	N2	NO	NO2	H2	S	SO2	SO3	H2S	H2O
.81E+01	.12E+02	.11E-03	.95E+00	.43E+02	.21E-02	.39E-05	.59E+01	.20E-01	.12E-04	.79E-08	.21E-02	.18E+02

HEAT OF REACTION= .111E+07
HEAT FOR TEMP RISE= .106E+07

FINAL DATA SUMMARY

FLAME TEMPERATURE = 2300.0 DEGREES FAHRENHEIT

HEAT OF REACTION= .111E+07
HEAT FOR TEMP RISE= .106E+07
THE FRESH FEED IS

C(S)	.81E+01	MOLES
O2	.12E+02	MOLES
CO	-0.	MOLES
CO2	-0.	MOLES
N2	.38E+02	MOLES

NO	-0.	MOLES
NO2	-0.	MOLES
H2	.59E+01	MOLES
S	.20E-01	MOLES
SO2	-0.	MOLES
SO3	-0.	MOLES
H2S	-0.	MOLES
H2O	.15E+02	MOLES

FINAL EQUILIBRIUM COMPOSITIONS

SPECIES SYMBOL	INITIAL MOLES	FINAL MOLES	CHANGE MOLES	GAS VOLUME	IDEAL VOLUME
C(S)	.814E+01	0.	.814E+01	0.	0.
O2	.118E+02	.660E+00	.111E+02	.293E+01	.570E+00
CO	.105E-03	.101E-02	-.904E-03	.448E-02	.871E-03
CO2	.947E+00	.909E+01	-.814E+01	.403E+02	.795E+01
N2	.426E+02	.426E+02	.881E-02	.189E+03	.368E+02
NO	.206E-02	.198E-01	-.177E-01	.877E-01	.171E-01
NO2	.390E-05	.374E-04	-.335E-04	.166E-03	.323E-04
H2	.594E+01	.376E-03	.594E+01	.167E-02	.325E-03
S	.202E-01	.166E-02	.185E-01	.738E-02	.144E-02
SO2	.123E-04	.118E-03	-.106E-03	.524E-03	.102E-03
SO3	.791E-08	0.	.791E-08	0.	0.
H2S	.214E-02	.205E-01	-.184E-01	.912E-01	.177E-01
H2O	.176E+02	.235E+02	-.592E+01	.104E+03	.203E+02

.59 (32) = 18.9
8.1 (44): 364.5
38 (28): 1063.
.018 (30): .54
.018 (34) .612
21 (18) 378.
1825.552

$\frac{.612}{1825.552}$: 335.5 ppm

NO 29.55 ppm
NO_2 .00034 (46) = .01564/.00856 .856 ppm
SO_2 .00704 3.85 ppm
SO_3 .0000044 .002405 ppm

BELOW ARE LISTED RESPECTIVELY, FOR EACH SPECIES, GRAM MOLES PURGED, AND STP VOLUME OF AMOUNTS PURGED AND RECYCLED.

C(S)	O2	CO	CO2	N2	NO	NO2	H2	S	SO2	SO3	H2S	H2O
.68E-07	.59E+00	.90E-03	.81E+01	.38E+02	.18E-01	.34E-04	.34E-03	.15E-02	.11E-03	.68E-07	.18E-01	.21E+02
.59E-07	.51E+00	.78E-03	.70E+01	.33E+02	.15E-01	.29E-04	.29E-03	.13E-02	.91E-04	.59E-07	.16E-01	.18E+02
.68E-08	.59E-01	.91E-04	.82E+00	.38E+01	.18E-02	.34E-05	.34E-04	.15E-03	.11E-04	.68E-08	.18E-02	.21E+01

THE TOTAL STP VOLUME TO BE PURGED IS .587E+02

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THE TOTAL STP VOLUME TO BE RECYCLED IS    .683E+01
 07/10/73 +SCOPE 3.3  VER 2.08 LEHIGH U. 06/13/73
12.25.44.TWASH78
12.25.44.TWASH,A3050,CM67000,T100,*HAWRYLO*,IDGAR
12.25.44.8,DPROB,P1.
12.25.45.FTN.
12.26.12.     9.027 CP SECONDS COMPILATION TIME
12.26.13.LGO.
12.27.00.EXIT
12.27.01.EXECUTION COST OF THIS JOB    $     4.17 (I/O COST NOT INCL)
12.27.01.PRIORITY SYSTEM RESOURCE UNITS     43.91
12.27.01.AUTHORIZED BALANCE IS         $  2190.38
12.27.01.CP      40.168 SEC.
12.27.01.PP      16.123 SEC.
        12.39.14.    TWASH78 001241 LINES PRINTED  /// END OF LIST ///   LP  22
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MMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMMM

(With Pure Oxygen Feed)

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      PROGRAM GARBAGE (INPUT, OUTPUT)
      EXTERNAL FNTX

C  NS IS THE NUMBER OF CHEMICAL SPECIES.
C  NREACT IS THE NUMBER OF REACTIONS.

C  THE REACTION OF C + 1/2 O2 FORMING CO MUST APPEAR AS THE FIRST RXN.
C   IN ACCOUNTING FOR LATENT HEAT OF VAPORIZATION OF WATER, IT HAS BEEN
C   NECESSARY TO STIPULATE THAT THE LAST CHEMICAL SPECIES MUST BE WATER.
C   YOU MUST HAVE WATER AS THE LAST CHEMICAL SPECIES OR CHANGE HVAP TO 0
C   HVAP IS IN CALORIES PER GRAM MOLE OF WATER.
C   RECYCLE RATIO IS DEFINED HERE AS THE RATIO OF MOLES OF RECYCLE GAS
C   TO THE MOLES OF FRESH FEED.
C   INITIAL AMOUNTS OF EACH SPECIES FED IN MUST BE GRAM MOLES.

      DIMENSION B(20),Z(20),Y(20),BV(20),BMIN(20),BMAX(20),P(400),A(20,2
     10),AC(20,20)
      DIMENSION BMI(20),BMA(20)
      DIMENSION SLOPE(20),YINTCP(20),HEAT(20)
      DIMENSION SENS2(20),VOL(20),VOLSTP(20)
      DIMENSION ALPHA(20),BETA(20),GAMMA(20),MARK(20),NPR(20)
      DIMENSION DELMOL(20),TGUESSF(40)
      DIMENSION BOX(20),NAME(20),RECY(20)
      DIMENSION FEED(20),RECYL(20),XXN(90,20)
      DIMENSION SPURGE(20),TSPVOL(20),TPEVOL(20)
      COMMON/TWO/XN(20),EQUIL(20),STOIC(20,20)
      COMMON/THREE/NS
      COMMON/FOUR/NSOL(20),GAS(20)

      JCOUNT=0
  --> RECYCLE=0.60
      PRINT 1
      READ 2,NS,NR
      NREACT = NR - 1

      READ 1500,(NAME(J),J=1,NS)
C     NSOL DESIGNATES IF SPECIAL CALCULATIONS REGARDING SOLID-GAS
C     REACTIONS ARE NECESSARY.
C     NSOL=1  MEANS COMPONENT IS A SOLID
C     NSOL=-1  MEANS COMPONENT IS GASEOUS
C     DATA REQUIREMENT---MUST WRITE REACTIONS SO THAT REACTIONS WITH
C     REACTANTS WHICH ARE PRODUCTS OF OTHER REACTIONS APPEAR AFTER ALL
C     THOSE REACTIONS.

C     DATA REQUIREMENT--CONCERNING THIS, THE REACTIONS MUST BE IN
C     IMMEDIATE SEQUENCE.
C     NPR=+1  MEANS THE COMPONENT APPEARS BOTH AS A PRODUCT AND A
C     REACTANT IN THE REACTION SYSTEM BEING STUDIED.
C     NPR=-1  MEANS THE COMPONENT APPEARS ONLY AS REACTANT IN THE
C     REACTION SYSTEM.
      DO 49 I = 1,NS
      READ 3, ALPHA(I), BETA(I), GAMMA(I), MARK(I), NSOL(I), NPR(I)
      PRINT 3003,ALPHA(I),BETA(I),GAMMA(I),MARK(I),NAME(I)
   49 CONTINUE
C  IF MARK IS NEGATIVE CP CONSTANTS FIT THE EQUATION CP = A + BT + C/T**2
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C  IF MARK IS POSITIVE THE EQUATION CP = A + BT + CT**2 IS USED.

PROGRAM    GARBAGE   TRACE                       CDC 6600 FTN V3.0-P336 OPT=0  07/09/73  10.39.01.     PAGE    2

          PRINT 1501,(NAME(J),J=1,NS)
          DO 50 J = 1,NREACT
          READ 14,(STOIC(J,I),I=1,NS)
          PRINT 4,(STOIC(J,I),I=1,NS)
       50 CONTINUE

C  THE LAST CARD (ROW) CONTAINS THE INITIAL NUMBER OF GRAM MOLES
C  FOR EACH SPECIES.
          READ 9,(STOIC(NR,I),I=1,NS)
          PRINT 1502,(NAME(J),J=1,NS)
          PRINT 3007,(STOIC(NR,I),I=1,NS)
          DO 61  J=1,NREACT
          READ 333,SLOPE(J),YINTCP(J),HEAT(J)
       61 CONTINUE
          TSUMT=0.0
          DO 7779 M=1,NS
          FEED(M)=STOIC(NR,M)
          TSUMT=TSUMT+FEED(M)
     7779 CONTINUE

          TREF = 298.0
C  T1 IS THE FEED TEMPERATURE.
          T1 = TREF
C  TGUESSF IS THE FLAME TEMPERATURE IN DEGREES FAHRENHEIT.
          JN=1
          TGUESSF(JN)=1940.00
     8999 CONTINUE
     7777 CONTINUE
          JCOUNT=JCOUNT+1
          K1=1
          PRINT 19285, TGUESSF(JN)
C  TGUESS IS IN DEGREES KELVIN.
          TGUESS=(TGUESSF(JN)-32.0)*5.0/9.0+273.1

          DO 60 J = 1,NREACT
          BMIN(J)=-1000.0
          BMAX(J)=+1000.0
          BV(J) = 1.0
       60 CONTINUE
          PRINT 3005

          IC = 0
          FNU=FLA=TAU=0.0
          EPS=FV=PHMIN=0.0
          NRR=NREACT-1
          ICON=NRR
          KD=NRR
          N=NRR
          KK=NRR
C  EQUIL(J) ARE THE EQUILIBRIUM CONSTANTS FOR EACH REACTION.
          DO 15 J = 1,NREACT
          EQUIL(J)=10.**(SLOPE(J)/TGUESS +YINTCP(J)  )
          Y(J) = 0.0
```

```
          INPUTC$      023573
          KODEP$       023727
          KRAKER$      025346
          OUTPTC$      027073
          ABS$         027167
          ALNLOGE      027172
          ALOG$        027231
          ATAN$        027263
          ATANE        027303
          EXPE         027364
          SQRT$        027430
          SQRTF        027454
          XTOY$        027476
          ----UNSATISFIED EXTERNALS-----                        REFERENCES

          .403E+01          .114E-02          -.204E+06          -1          C(S)
          .615E+01          .310E-02          -.923E-06           1          O2
          .642E+01          .166E-02          -.196E-06           1          CO
          .621E+01          .104E-01          -.354E-05           1          CO2
          .683E+01          .900E-03          -.120E+05          -1          N2
          .703E+01          .920E-03          -.140E+05          -1          NO
          .101E+02          .228E-02          -.167E+06          -1          NO2
          .652E+01          .780E-03           .120E+05          -1          H2
          .526E+01         -.100E-03           .360E+05          -1          S
          .110E+02          .188E-02          -.184E+06          -1          SO2
          .139E+02          .610E-02          -.322E+06          -1          SO3
          .666E+01          .513E-02          -.854E-06           1          H2S
          .730E+01          .246E-02          0.                 -1          H2O
   C(S)   O2    CO    CO2   N2    NO    NO2   H2    S     SO2   SO3   H2S   H2O
   -1.0   -.5   1.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0
   -0.0   -.5  -1.0   1.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0
   -0.0   -.5  -0.0  -0.0   -.5   1.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0
   -0.0   -.5  -0.0  -0.0  -0.0  -1.0   1.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0
   -0.0   -.5  -0.0  -0.0  -0.0  -0.0  -0.0  -1.0  -0.0  -0.0  -0.0  -0.0   1.0
   -0.0  -1.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -1.0   1.0  -0.0  -0.0  -0.0
   -0.0   -.5  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -1.0   1.0  -0.0  -0.0
   -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -0.0  -1.0  -1.0  -0.0  -0.0   1.0  -0.0
    C(S)     O2       CO       CO2      N2      NO       NO2      H2      S      SO2      SO3      H2S      H2O

   8.140  11.700  -0.000  -0.000    .300  -0.000  -0.000   5.940   .020  -0.000  -0.000  -0.000  15.160
          TGUESSF=     1940.00
```

Output

```
                                 EQUILIBRIUM CONSTANTS
   .122E+18     .267E+07     .135E-02     .436E-01     .711E+07     .843E+01     .283E-02     .768E+07

  BMIN(J)=       -0.00000000   BMAX(J)=         8.14000000
  BMIN(J)=       -0.00000000   BMAX(J)=         8.14000000
  BMIN(J)=       -0.00000000   BMAX(J)=          .60000000
  BMIN(J)=       -0.00000000   BMAX(J)=          .60000000
  BMIN(J)=      -15.16000000   BMAX(J)=         5.94000000
  BMIN(J)=       -0.00000000   BMAX(J)=          .02000000
  BMIN(J)=       -0.00000000   BMAX(J)=          .02000000
  BMIN(J)=       -0.00000000   BMAX(J)=          .02000000
    1.     7 0.       0.       0.       0.       0.       0.       0.       .2E+04
    9.     7  .6E-04  .2E-04  .8E-05  .6E+01  .2E-04  .6E-05  .3E-04  .8E+03
   17.     7  .2E-02  .2E-03  .2E-04  .6E+01  .2E-03  .2E-04  .3E-03  .7E+03
   25.     7  .4E-01  .6E-03  .3E-04  .6E+01  .1E-02  .2E-04  .2E-02  .4E+03
   33.     7  .8E+00  .1E-02  .2E-04  .6E+01  .4E-02  .8E-05  .6E-02  .3E+03
   41.     7  .8E+01  .7E-03-0.       .6E+01  .2E-02-0.       .1E-01  .2E+03
   59.     6  .8E+01  .7E-03  .8E-07  .6E+01  .1E-02  .5E-07  .1E-01  .1E+03
   67.     6  .8E+01  .6E-03  .8E-06  .6E+01  .1E-02  .5E-06  .2E-01  .1E+03
   76.     7  .8E+01  .6E-03  .1E-05  .6E+01  .1E-02  .5E-06  .2E-01  .7E+02
   86.     4  .8E+01  .6E-03  .1E-05  .6E+01  .1E-02  .5E-06  .2E-01  .6E+02
   95.     4  .8E+01  .5E-03  .1E-05  .6E+01  .1E-02  .5E-06  .2E-01  .6E+02
  104.     4  .8E+01  .5E-03  .1E-05  .6E+01  .1E-02  .5E-06  .2E-01  .6E+02
  113.     4  .8E+01  .5E-03  .1E-05  .6E+01  .1E-02  .5E-06  .2E-01  .6E+02
  122.     4  .8E+01  .5E-03  .2E-05  .6E+01  .1E-02  .5E-06  .2E-01  .6E+02
  131.     4  .8E+01  .5E-03  .2E-05  .6E+01  .1E-02  .5E-06  .2E-01  .6E+02
  140.     4  .8E+01  .5E-03  .2E-05  .6E+01  .1E-02  .5E-06  .2E-01  .5E+02
  149.     4  .8E+01  .5E-03  .2E-05  .6E+01  .1E-02  .5E-06  .2E-01  .5E+02
  158.     4  .8E+01  .5E-03  .2E-05  .6E+01  .1E-02  .5E-06  .2E-01  .5E+02
  167.     4  .8E+01  .5E-03  .2E-05  .6E+01  .1E-02  .5E-06  .2E-01  .5E+02
  175.     4  .8E+01  .5E-03  .2E-05  .6E+01  .1E-02  .6E-06  .2E-01  .5E+02
  183.     7  .8E+01  .5E-03  .3E-05  .6E+01  .1E-02  .1E-06  .2E-01  .4E+02
  194.     4  .8E+01  .5E-03  .3E-05  .6E+01  .1E-02  .1E-06  .2E-01  .4E+02
  203.     4  .8E+01  .5E-03  .3E-05  .6E+01  .1E-02  .2E-06  .2E-01  .4E+02
  212.     4  .8E+01  .5E-03  .3E-05  .6E+01  .1E-02  .2E-06  .2E-01  .4E+02
  221.     3  .8E+01  .5E-03  .3E-05  .6E+01  .1E-02  .2E-06  .2E-01  .4E+02
  230.     3  .8E+01  .5E-03  .3E-05  .6E+01  .1E-02  .2E-06  .2E-01  .3E+02
  239.     3  .8E+01  .5E-03  .3E-05  .6E+01  .1E-02  .2E-06  .2E-01  .3E+02
  248.     3  .8E+01  .5E-03  .3E-05  .6E+01  .1E-02  .2E-06  .2E-01  .3E+02
  257.     3  .8E+01  .5E-03  .3E-05  .6E+01  .1E-02  .3E-06  .2E-01  .3E+02
  266.     3  .8E+01  .5E-03  .3E-05  .6E+01  .1E-02  .3E-06  .2E-01  .3E+02
  275.     3  .8E+01  .5E-03  .3E-05  .6E+01  .1E-02  .3E-06  .2E-01  .3E+02
  284.     3  .8E+01  .5E-03  .3E-05  .6E+01  .1E-02  .3E-06  .2E-01  .2E+02
  293.     3  .8E+01  .5E-03  .3E-05  .6E+01  .1E-02  .3E-06  .2E-01  .2E+02
  302.     3  .8E+01  .5E-03  .3E-05  .6E+01  .1E-02  .3E-06  .2E-01  .2E+02
     -.69E+00      -.13E+00       .20E-01      -.36E+01       .15E+01      -.25E+00      -.24E+01

               8.140000  =  EXTENT OF REACTION   1

               8.139957  =  EXTENT OF REACTION   2

                .000506  =  EXTENT OF REACTION   3

                .000003  =  EXTENT OF REACTION   4

               5.921222  =  EXTENT OF REACTION   5
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                  .000972  = EXTENT OF REACTION   6

                  .000000  = EXTENT OF REACTION   7

                  .018029  = EXTENT OF REACTION   8
 PRODUCTS OF THE REACTIONS ARE AS FOLLOWS
    C(S)      O2        CO       CO2       N2        NO        NO2       H2        S         SO2       SO3       H2S       H2O
 0.        .60E+00   .43E-04   .81E+01   .30E+00   .50E-03   .31E-05   .75E-03   .10E-02   .97E-03   .30E-06   .18E-01   .21E+02

   AMOUNTS OF EACH SPECIES TO BE RECYCLED
 .25E-07   .49E+00   .35E-04   .67E+01   .25E+00   .41E-03   .26E-05   .62E-03   .82E-03   .80E-03   .25E-06   .15E-01   .17E+02
 MOLES TO BE PURGED =      .54E+01
          HEAT OF REACTION=    .111E+07
          HEAT FOR TEMP RISE=    .516E+06
                              COMPOSITION AFTER CYCLE     1
                              NUMBER OF SATISFIED COMPONENTS        0

              THE TOTAL FEED IS

    C(S)      O2        CO       CC2       N2        NO        NO2       H2        S         SO2       SO3       H2S       H2O
 .81E+01   .12F+02   .35E-04   .67E+01   .55E+00   .41E-03   .26E-05   .59E+01   .21E-01   .80E-03   .25E-06   .15E-01   .32E+02

          TGUESSF=     1940.00



                              EQUILIBRIUM CONSTANTS
    .122E+10    .267E+07    .135E-C2    .436E-01    .711E+07    .843E+01    .283E-02    .768E+07
 BMIN(J)=        -.00003538   BMAX(J)=        8.14000002
 BMIN(J)=       -6.68580113   BMAX(J)=        8.14003541
 BMIN(J)=        -.00041298   BMAX(J)=        1.09239793
 BMIN(J)=        -.00000259   BMAX(J)=        1.09281092
 BMIN(J)=      -32.47518434   BMAX(J)=        5.94061539
 BMIN(J)=        -.00079799   BMAX(J)=         .02082046
 BMIN(J)=        -.00000025   BMAX(J)=         .02161845
 BMIN(J)=        -.01480842   BMAX(J)=         .02082046
    1.    7  0.       0.       0.        0.       0.        0.        0.       .6E+03
    9.    7  .8E+01 -.4E-03 -.3E-05  .6E+01 -.8E-03 -.2E-06  .2E-01  .3E+03
   20.    6  .8E+01 -.4E-03 -.3E-06  .6F+01 -.8E-03  .2E-05  .2E-01  .2E+03
   30.    7  .8E+01 -.3E-03 -.3E-05  .6E+01 -.7E-03 -.2E-06  .1E-01  .1E+03
   41.    5  .8E+01 -.3E-03 -.3E-05  .6E+01 -.7E-03 -.2E-06  .9E-02  .9E+02
   49.    5  .8E+01 -.3E-03 -.2E-05  .6E+01 -.7E-03 -.2E-05  .1E-01  .6E+02
   58.    5  .8E+01 -.3E-03 -.2E-05  .6E+01 -.7E-03 -.2E-06  .1E-01  .5E+02
   68.    3  .8E+01 -.3E-03 -.2E-05  .6F+01 -.7E-03 -.2E-06  .1E-01  .5E+02
   77.    3  .8E+01 -.3E-03 -.2E-05  .6E+01 -.7E-03 -.2E-05  .1E-01  .5E+02
   86.    3  .8E+01 -.3E-03 -.2E-05  .6E+01 -.7E-03 -.2E-06  .1E-01  .5E+02
   94.    5  .8E+01 -.3E-03 -.2E-05  .6E+01 -.7E-03 -.2E-06  .1E-01  .4E+02
  103.    5  .8E+01 -.3E-03 -.2F-05  .6F+01 -.7F-03 -.2E-06  .1E-01  .3E+02
  113.    3  .8E+01 -.3E-03 -.2E-05  .6E+01 -.7E-03 -.2E-06  .1E-01  .3E+02
  122.    3  .8E+01 -.3E-03 -.2E-05  .6E+01 -.7E-03 -.2E-06  .1E-01  .3E+02
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131.   3  .8E+01 -.3E-03 -.2E-05  .6E+01 -.7E-03 -.2E-06  .1E-01  .3E+02
140.   3  .8E+01 -.3E-03 -.2E-05  .6E+01 -.7E-03 -.2E-06  .1E-01  .2E+02
149.   3  .8E+01 -.3E-03 -.2E-05  .6E+01 -.7E-03 -.2E-06  .1E-01  .2E+02
158.   3  .8E+01 -.3E-03 -.2E-05  .6E+01 -.7E-03 -.2E-06  .1E-01  .2E+02
166.   6  .8E+01 -.3E-03 -.2E-05  .6E+01 -.6E-03 -.2E-06  .1E-01  .2E+02
175.   5  .8E+01 -.3E-03 -.2E-05  .6E+01 -.6E-03 -.2E-06  .1E-01  .1E+02
185.   3  .8E+01 -.3E-03 -.2E-05  .6E+01 -.6E-03 -.2E-06  .1E-01  .1E+02
194.   3  .8E+01 -.3E-03 -.2E-05  .6E+01 -.6E-03 -.2E-06  .1E-01  .9E+01
203.   2  .8E+01 -.3E-03 -.2E-05  .6E+01 -.6E-03 -.2E-06  .1E-01  .8E+01
212.   2  .8E+01 -.3E-03 -.2E-05  .6E+01 -.6E-03 -.2E-06  .1E-01  .8E+01
221.   2  .8E+01 -.3E-03 -.2E-05  .6E+01 -.6E-03 -.2E-06  .1E-01  .8E+01
230.   2  .8E+01 -.3E-03 -.2E-05  .6E+01 -.6E-03 -.2E-06  .1E-01  .7E+01
239.   2  .8E+01 -.3E-03 -.2E-05  .6E+01 -.6E-03 -.2E-06  .1E-01  .7E+01
247.   5  .8E+01 -.3E-03 -.2E-05  .6E+01 -.6E-03 -.2E-06  .1E-01  .7E+01
256.   4  .8E+01 -.2E-03 -.2E-05  .6E+01 -.6E-03 -.2E-06  .1E-01  .7E+01
266.   2  .8E+01 -.2E-03 -.2E-05  .6E+01 -.6E-03 -.2E-06  .1E-01  .7E+01
275.   2  .8E+01 -.2E-03 -.2E-05  .6E+01 -.6E-03 -.2E-06  .1E-01  .6E+01
284.   2  .8E+01 -.2E-03 -.2E-05  .6E+01 -.6E-03 -.2E-06  .1E-01  .6E+01
293.   2  .8E+01 -.2E-03 -.2E-05  .6E+01 -.6E-03 -.2E-06  .1E-01  .6E+01
302.   2  .8E+01 -.2E-03 -.2E-05  .6E+01 -.6E-03 -.2E-06  .1E-01  .6E+01
   -.25E+00     -.17E+01      -.18E+00      .28E-01      -.16E+01      -.51E-01      -.19E+00

                 8.140000  = EXTENT OF REACTION  1

                 8.139985  = EXTENT OF REACTION  2

                 -.000233  = EXTENT OF REACTION  3

                 -.000002  = EXTENT OF REACTION  4

                 5.926001  = EXTENT OF REACTION  5

                 -.000569  = EXTENT OF REACTION  6

                 -.000000  = EXTENT OF REACTION  7

                  .014577  = EXTENT OF REACTION  8

 PRODUCTS OF THE REACTIONS ARE AS FOLLOWS

   C(S)      O2       CO       CO2       N2       NO       NO2       H2        S        SO2       SO3       H2S       H2O
 0.       .11E+01  .51E-04  .15E+02  .55E+00  .18E-03  .93E-06  .37E-04  .68E-02  .23E-03  .87E-07  .29E-01  .38E+02

  AMOUNTS OF EACH SPECIES TO BE RECYCLED
 .25E-07  .49E+00  .23E-04  .67E+01  .25E+00  .82E-04  .42E-06  .17E-04  .31E-02  .10E-03  .39E-07  .13E-01  .17E+02

 MOLES TO BE PURGED =     .30E+02
        HEAT OF REACTION=    .111E+07
        HEAT FOR TEMP RISE=    .941E+06
                        COMPOSITION AFTER CYCLE     2
                        NUMBER OF SATISFIED COMPONENTS     13

            THE TOTAL FEED IS

   C(S)      O2       CO       CO2       N2       NO       NO2       H2        S        SO2       SO3       H2S       H2O
 .81E+01  .12E+02  .23E-04  .67E+01  .55E+00  .82E-04  .42E-06  .59E+01  .23E-01  .10E-03  .39E-07  .13E-01  .32E+02
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HEAT OF REACTION=    .111E+07
HEAT FOR TEMP RISE=    .941E+06
TGUESSF=     2270.00

                         EQUILIBRIUM CONSTANTS
  .358E+09    .124E+06    .361E-02    .215E-01    .471E+06    .176E+01    .241E-03    .463E+07

BMIN(J)=        -.00002279   BMAX(J)=        8.14000002
BMIN(J)=       -6.68549808   BMAX(J)=        8.14002282
BMIN(J)=        -.00008201   BMAX(J)=        1.09270780
BMIN(J)=        -.00000042   BMAX(J)=        1.09278981
BMIN(J)=      -32.47652199   BMAX(J)=        5.94001683
BMIN(J)=        -.00016330   BMAX(J)=         .02307187
BMIN(J)=        -.00000004   BMAX(J)=         .02317517
BMIN(J)=        -.01325113   BMAX(J)=         .02307187
   1.    7 0.        0.        0.        0.        0.        0.        0.        .4E+03
   9.    7  .8E+01   .2E-03    .2E-05    .6E+01  -.1E-03   -.4E-07    .2E-01    .4E+03
  19.    7  .8E+01   .3E-02    .8E-04   -.2E+02  -.5E-04    .4E-04    .2E-01    .4E+03
  31.    7  .8E+01   .3E-02    .7E-04   -.1E+02  -.5E-04    .4E-04    .2E-01    .4E+03
  40.    7  .8E+01   .3E-02    .6E-04   -.4E+01  -.4E-04    .3E-04    .2E-01    .3E+03
  48.    6  .8E+01   .4E-02    .6E-05    .6E+01  -.2E-05   -.4E-07    .2E-01    .2E+03
  57.    6  .8E+01   .4E-02    .1E-04    .3E+01  -.6E-04   -.4E-07    .2E-01    .2E+03
  67.    6  .8E+01   .3E-02    .1E-04    .4E+01  -.6E-04   -.4E-07    .2E-01    .1E+03
  76.    5  .8E+01   .3E-02    .1E-04    .5E+01  -.5E-04   -.4E-07    .2E-01    .1E+03
  85.    5  .8E+01   .3E-02    .1E-04    .5E+01  -.5E-04   -.4E-07    .2E-01    .9E+02
  94.    5  .8E+01   .3E-02    .1E-04    .6E+01  -.5E-04   -.4E-07    .2E-01    .7E+02
 103.    5  .8E+01   .3E-02    .1E-04    .6E+01  -.5E-04   -.4E-07    .2E-01    .6E+02
 112.    5  .8E+01   .3E-02    .1E-04    .6E+01  -.5E-04   -.4E-07    .2E-01    .5E+02
 121.    4  .8E+01   .3E-02    .1E-04    .6E+01  -.4E-04   -.4E-07    .2E-01    .5E+02
 130.    5  .8E+01   .3E-02    .1E-04    .6E+01  -.4E-04   -.4E-07    .2E-01    .4E+02
 139.    5  .8E+01   .3E-02    .1E-04    .6E+01  -.4E-04   -.4E-07    .2E-01    .4E+02
 148.    5  .8E+01   .3E-02    .1E-04    .6E+01  -.4E-04   -.4E-07    .2E-01    .3E+02
 157.    5  .8E+01   .3E-02    .1E-04    .6E+01  -.4E-04   -.4E-07    .2E-01    .3E+02
 166.    5  .8E+01   .3E-02    .1E-04    .6E+01  -.4E-04   -.4E-07    .2E-01    .3E+02
 174.    5  .8E+01   .3E-02    .1E-04    .6E+01  -.6E-04   -.4E-07    .2E-01    .2E+02
 182.    4  .8E+01   .3E-02    .8E-05    .6E+01  -.8E-04   -.4E-07    .2E-01    .2E+02
 191.    5  .8E+01   .3E-02    .8E-05    .6E+01  -.8E-04   -.4E-07    .2E-01    .2E+02
 200.    6  .8E+01   .3E-02    .8E-05    .6E+01  -.7E-04   -.4E-07    .2E-01    .2E+02
 209.    6  .8E+01   .3E-02    .8E-05    .6E+01  -.7E-04   -.4E-07    .2E-01    .1E+02
 219.    4  .8E+01   .3E-02    .8E-05    .6E+01  -.5E-04   -.4E-07    .2E-01    .1E+02
 228.    4  .8E+01   .3E-02    .8E-05    .6E+01  -.3E-04   -.4E-07    .2E-01    .1E+02
 237.    4  .8E+01   .3E-02    .8E-05    .6E+01  -.2E-04   -.4E-07    .2E-01    .1E+02
 246.    4  .8E+01   .3E-02    .8E-05    .6E+01  -.4E-05   -.4E-07    .2E-01    .9E+01
 256.    4  .8E+01   .3E-02    .8E-05    .6E+01   .2E-05   -.4E-07    .2E-01    .9E+01
 264.    4  .8E+01   .3E-02    .8E-05    .6E+01   .7E-05   -.4E-07    .2E-01    .9E+01
 273.    4  .8E+01   .3E-02    .8E-05    .6E+01   .1E-04   -.4E-07    .2E-01    .8E+01
 283.    3  .8E+01   .3E-02    .8E-05    .6E+01   .2E-04   -.4E-07    .2E-01    .8E+01
 291.    4  .8E+01   .3E-02    .8E-05    .6E+01   .2E-04   -.4E-07    .2E-01    .8E+01
 300.    4  .8E+01   .3E-02    .8E-05    .6E+01   .2E-04   -.4E-07    .2E-01    .8E+01
 309.    4  .8E+01   .3E-02    .8E-05    .6E+01   .2E-04   -.4E-07    .2E-01    .8E+01
      .37E+00      -.22E-02      .23E-04      .20E+00      .11E+01      .25E+01      -.28E+00

          8.140000  = EXTENT OF PEACTION   1
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8.139436 = EXTENT OF REACTION 2

.002702 = EXTENT OF PEACTION 3

.000008 = EXTENT OF PEACTION 4

5.917664 = EXTENT OF PEACTION 5

.000023 = EXTENT OF REACTION 6

-.000000 = EXTENT OF PEACTION 7

.021881 = EXTENT OF PEACTION 8

PRODUCTS OF THE REACTIONS ARE AS FOLLOWS

C(S)	O2	CO	CO2	N2	NO	NO2	H2	S	SO2	SO3	H2S	H2O
0.	.11F+C1	.59E-03	.15E+C2	.55E+C0	.25E-02	.84E-05	.47E-03	.12E-02	.13E-03	0.	.35E-01	.38E+02

AMOUNTS OF EACH SPECIES TO BE RECYCLED

.25E-07	.49E+00	.26E-03	.67E+01	.25E+C0	.13E-02	.39E-05	.21E-03	.53E-03	.57E-04	.25E-07	.16E-01	.17E+C2

MOLES TO BE PURGED = .30E+02
HEAT OF REACTION= .111E+07
HEAT FOR TEMP PISE= .106E+C7
COMPOSITION AFTER CYCLE 3
NUMBER OF SATISFIED COMPONENTS 13

THE TOTAL FEED IS

C(S)	O2	CO	CC2	N2	NO	NO2	H2	S	SO2	SO3	H2S	H2O
.81E+01	.12E+02	.26E-03	.67E+01	.55E+C0	.13E-02	.39E-05	.59E+01	.21E-01	.57E-04	.25E-07	.16E-01	.32E+02

HEAT OF REACTION= .111E+07
HEAT FOR TEMP PISE= .106E+C7

FINAL DATA SUMMARY

FLAME TEMPERATURE = 2270.0 DEGPEES FAHRENHEIT

HEAT OF REACTION= .111E+C7
HEAT FOR TEMP RISE= .106E+C7
THF FRESH FEED IS
C(S) .81E+01 MOLES
O2 .12E+02 MOLES
CO -0. MOLES
CO2 -0. MOLFS
N2 .30E+00 MOLES

NO	-0.	MOLES
NO2	-0.	MOLES
H2	.59E+01	MOLES
S	.20E-01	MOLES
SO2	-0.	MOLES
SO3	-0.	MOLES
H2S	-0.	MOLES
H2O	.15E+02	MOLES

FINAL EQUILIBRIUM COMPOSITIONS

SPECIES SYMBOL	INITIAL MOLES	FINAL MOLES	CHANGE MOLES	GAS VOLUME	IDEAL VOLUME
C(S)	.814E+01	0.	.814E+01	0.	0.
O2	.122E+02	.109E+01	.111E+02	.479E+01	.942E+00
CO	.265E-03	.587E-03	-.322E-03	.258E-02	.507E-03
CO2	.669E+01	.148E+02	-.814E+01	.651E+02	.128E+02
N2	.546E+00	.545E+00	.775E-03	.239E+01	.471E+00
NO	.125E-02	.278E-02	-.152E-02	.122E-01	.240E-02
NO2	.379E-05	.841E-05	-.462E-05	.369E-04	.726E-05
H2	.594E+01	.472E-03	.594E+01	.207E-02	.408E-03
S	.205E-01	.117E-02	.194E-01	.513E-02	.101E-02
SO2	.571E-04	.127E-03	-.695E-04	.556E-03	.109E-03
SO3	.248E-07	0.	.248E-07	0.	0.
H2S	.158E-01	.351E-01	-.193E-01	.154E+00	.303E-01
H2O	.325E+02	.384E+02	-.592E+01	.169E+03	.332E+02

BELOW ARE LISTED RESPECTIVELY, FOR EACH SPECIES, GRAM MOLES PURGED, AND STP VOLUME OF AMOUNTS PURGED AND RECYCLED.

C(S)	O2	CO	CO2	N2	NO	NO2	H2	S	SO2	SO3	H2S	H2O
.30E-07	.60E+00	.32E-03	.81E+01	.30E+00	.15E-02	.46E-05	.26E-03	.64E-03	.69E-04	.30E-07	.19E-01	.21E+02
.26E-07	.52E+00	.28E-03	.70E+01	.26E+00	.13E-02	.40E-05	.22E-03	.55E-03	.60E-04	.26E-07	.17E-01	.18E+02
.21E-07	.42F+00	.23E-03	.58E+01	.21E+00	.11E-02	.33E-05	.18E-03	.45E-03	.49E-04	.21E-07	.14E-01	.15E+02

THE TOTAL STP VOLUME TO BE PURGED IS .260E+02

.019(34) = .641
21(18) 378.
.3(20) F.4

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THE TOTAL STP VOLUME TO BE RECYCLED IS     .214E+02
 07/09/73  SCOPE 3.3  VER 2.08 LEHIGH U. 06/13/73
10.38.58.TWASH53
10.38.58.TWASH,A3050,CM67300,T100,*HAWRYLO*,IDGAR
10.38.58.B,DPROB,P1.
10.38.59.FTN.
10.39.29.      9.019 CP SECONDS COMPILATION TIME
10.39.29.LGO.
10.40.31.EXIT
10.40.32.EXECUTION COST OF THIS JOB     $      4.02 (I/O COST NOT INCL)
10.40.32.PRIORITY SYSTEM RESOURCE UNITS      42.31
10.40.32.AUTHORIZED BALANCE IS          $  2236.95
10.40.32.CP      39.886 SEC.
10.40.32.PP      12.401 SEC.
      10.41.41.    TWAS453 001241 LINES PRINTED  /// END OF LIST ///   LP  23
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$\frac{1.2}{762.746}$

$\frac{.646}{762.746} = .847 \times 10^{-6}$

$.0015 (30) = .045$

$.0000046 (46) = .000212$

$.000069 (64) = .00442$

$.0000003 (50) = .000024$

Footnotes

1. Marquardt, D., "An Algorithm for Least-Squares Estimation of Nonlinear Parameters," Journal for the Society of Industrial and Applied Mathematics, Vol. 11, No. 2, June 1963, pg. 431-441.

2. Henley and Rosen, Material and Energy Balance Computations, John Wiley & Sons, Inc., New York, 1969.

3. Chien and Sanderson, Industrial & Engineering Chemistry Process Design & Development, Vol. 12, 1973, pg. 81.

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